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DYNAMIC MODELS OF BINARY PLATE DISTILLATION

by

Michael Ney Hayes

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by

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(1965)

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at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

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Submitted to the Department of Electrical Engineering on August 18, 1969

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ABSTRACT

This thesis investigates continuous-spatial dynamic models of the composition behavior of binary plate distillation columns. These partial differential equation models are developed from basic distillation column principles and the discrete-plate models by treating the plate number as a continuous-spatial variable. Linearized continuous-spatial models are investigated in detail.

The central purpose of this thesis is the development, presentation, suggested analytical solution technique, and example column evaluation of the Linear Polynomial-Coefficient Model (LPCM) which is a linearized continuous-spatial model in which the coefficients in the partial differential equation are n-th degree polynomials in the spatial variable. A general analytical solution technique is proposed in which the spatial differential eigenvalue problem resulting from separation of variables is transformed to a Liouville Normal-Form equation which is then converted to a homogeneous Fredholm II integral equation. Several simple examples of the model are solved in complete detail, and the proposed solution technique is applied to a model with first-degree polynomial coefficients. An analytical and a computational analysis giving the details of each step of the solution technique is presented. It is suggested that greatly reduced computation times compared to discrete models will result from application of the proposed solution technique.

A bibliography of 352 references, 202 of which pertain directly to distillation column dynamics and control, is presented and related to the areas of the thesis.

Thesis Supervisor: Lawrence B. Evans

Title: Associate Professor of Chemical Engineering

ACKNOWLEDGEMENT

THE AUTHOR WISHES TO THANK THE UNITED STATES NAVY FOR ITS SUPPORT THROUGHOUT HIS SERVICE, UNDERGRADUATE, AND GRADUATE EDUCATIONS. THIS SUPPORT CAME IN THE FORM OF FINANCIAL COVERAGE OF THE AUTHOR'S EDUCATION AND PERSONAL SUPPORT FROM THE MANY OUTSTANDING MEN WITH WHOM HE HAD HAD THE PRIVILEGE OF WORKING.

THE AUTHOR IS ALSO INDEBTED TO PROF. LEONARD A. GOULD, ELECTRICAL ENGINEERING DEPARTMENT, FOR SUGGESTING AN APPROXIMATION TECHNIQUE WHICH LED THE AUTHOR INTO THIS THESIS AND TO THE DEVELOPMENT OF THE LINEAR POLYNOMIAL-COEFFICIENT MODEL PRESENTED THEREIN.

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FINALLY, THE AUTHOR EXPRESSES HIS APPRECIATION FOR THE COMPUTATION FUNDS SUPPLIED BY THE M.I.T. DEPT. OF ELECTRICAL ENGINEERING.

THESIS FORMAT AND MNEMONICS

SECTION	MNEMONIC LETTER	TITLE
0	C	CONTENTS AND ARRANGEMENT OF THESIS
1	I	INTRODUCTION TO DISTILLATION
2	M	MODELS OF BINARY DISTILLATION COLUMNS
3	L	LINEAR POLYNOMIAL - COEFFICIENT MODEL (LPCM)
4	S	SUMMARY AND CONCLUSION
5	A	APPENDICES
6	B	BIBLIOGRAPHY AND REFERENCING

ALL CHAPTERS, SUBSECTIONS, TABLES, ILLUSTRATIONS, AND EQUATIONS IN THIS THESIS WILL BE IDENTIFIED IN THE ORDER:

MNEMONIC LETTER CHAPTER NUMBER . ORDINAL NUMBER .

FOR EXAMPLE: EQUATION L1.1, THE CENTRAL EQUATION OF THIS THESIS, IS LOCATED IN SECTION 3, CHAPTER 1 AND IS THE FIRST EQUATION IN THAT CHAPTER. REMEMBERING THE MEANING OF L, THE READER KNOWS, WITHOUT LOOKING IT UP, THAT L1.1, WHEREVER IT APPEARS, IS PART OF THE LPCM.

ALL BIBLIOGRAPHY REFERENCES ARE IN PARENTHESIS AND ARE IN THE ORDER:

(FIRST LETTER OF AUTHOR'S LAST NAME - SEQUENCE NUMBER)

SECTION 0

CONTENTS AND ARRANGEMENT OF THESIS (C)

C1 TABLE OF CONTENTS

C2 CHAPTER AND APPENDIX RELATIONSHIP DIAGRAM

C3 LIST OF TABLES

C4 LIST OF ILLUSTRATIONS

"EVERY INVESTIGATION WHICH IS GUIDED BY PRINCIPLES OF NATURE FIXES ITS ULTIMATE AIM ENTIRELY ON GRATIFYING THE STOMACH." —

ATHENAEUS, 200 A.D.

CHAPTER C1

TABLE OF CONTENTS

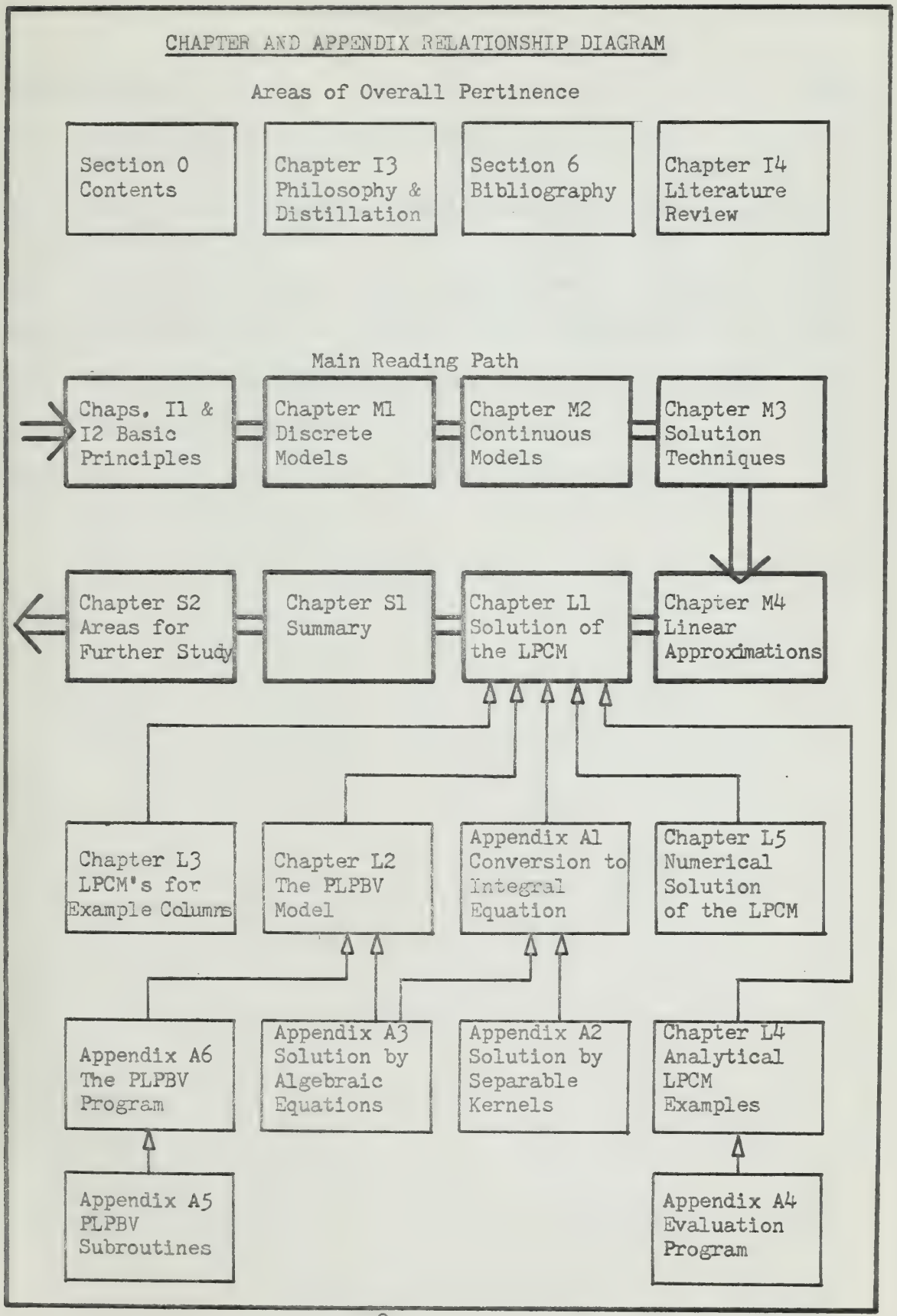
TABLE OF CONTENTS (CONTD.)

CHAPTER C2

CHAPTER AND APPENDIX RELATIONSHIP DIAGRAM

For the convenience of the reader this chapter presents in flowchart form a diagram relating all of the 28 chapters and appendices presented in the Table of Contents. The author hopes that this diagram will aid the reader in quickly establishing a sense of the structure of this thesis.

This diagram represents a combination of reading path and application relationships. The arrows from one box to the next imply reading direction and dependence direction. For example, the main reading path through the thesis has been designed as I1, I2, M1, M2, M3, M4, L1, S1, S2; the other chapters which consider subcases and solutions of these are shown leading into the main reading path which is in double black lines.


CHAPTER AND APPENDIX RELATIONSHIP DIAGRAM
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Main Reading Path
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SECTION 1

INTRODUCTION TO DISTILLATION (I)

I1 BASIC PRINCIPLES OF BINARY DISTILLATION

I2 THE BINARY PLATE DISTILLATION COLUMN

I3 PHILOSOPHY AND DISTILLATION

I4 A BRIEF REVIEW OF THE LITERATURE OF DISTILLATION

THE FUNDAMENTAL AND UNIVERSAL ABSOLUTE:

"EXISTENCE, REALITY, THE EXTERNAL WORLD, IS WHAT IT IS, INDEPENDENT OF MAN'S CONSCIOUSNESS, INDEPENDENT OF ANYONE'S KNOWLEDGE, JUDGMENT, BELIEFS, HOPES, WISHES, OR FEARS — THAT FACTS ARE FACTS, THAT A IS A, THAT THINGS ARE WHAT THEY ARE."

NATHANIEL BRANDEN (B-28)

THIS SECTION PRESENTS THE BASIC PHYSICAL AND MATHEMATICAL IDEAS OF BINARY DISTILLATION ORIENTED TOWARD FORMING A MATHEMATICAL MODEL OF A BINARY PLATE DISTILLATION COLUMN. THE GENERAL PROBLEM OF OBSERVING AND MODELING PHYSICAL SYSTEMS IS DISCUSSED AND THE HISTORY AND GENERAL LITERATURE OF DISTILLATION ARE REVIEWED BRIEFLY. SEVERAL OPINIONS ON THE PHILOSOPHY OF OBSERVING REALITY AS RELATED TO MODELING A DISTILLATION COLUMN AND ON THE DESIRE TO ACHIEVE PROFIT AS RELATED TO THE COST OF SEPARATION OF COMPONENTS ARE PRESENTED.

THE CENTRAL PURPOSE OF THIS THESIS IS THE DEVELOPMENT, PRESENTATION, SUGGESTED SOLUTION TECHNIQUE, AND EVALUATION OF THE LINEAR POLYNOMIAL-COEFFICIENT MODEL (LPCM) OF THE DYNAMIC BEHAVIOR OF A BINARY PLATE DISTILLATION COLUMN. THIS SECTION PRESENTS THE BASIC PRINCIPLES LEADING UP TO THE COMPLETE DEVELOPMENT OF THE LPCM IN SECTION 2(M) AND THE PRESENTATION OF AN INTEGRAL EQUATION SOLUTION TECHNIQUE IN SECTION3(L).

CHAPTER I1

BASIC PRINCIPLES OF BINARY DISTILLATION

The purpose of Chapters I1 and I2 is to present the basic principles behind the separation of binary mixtures and to develop the techniques for describing mathematically and graphically the steady state characteristics of a distillation column. These topics are presented for several reasons:

1. Some readers may not be acquainted with the basic theory, which is necessary for the developments which follow.

2. This is a convenient method for developing a consistent notation for use throughout this thesis.

3. Presentations of those basic principles specifically used in this thesis are not often found in the existing literature in forms easily understood by readers without some background in the subject.

There are many available techniques for describing binary distillation in quantitative or qualitative terms. Most of these techniques are oriented specifically toward one of these two outlooks. The technique to be described in Chapters I1 and I2 is the use of the McCabe-Thiele diagram which has the unique advantage of a quantitative, qualitative, and, in a sense, visual insight into binary distillation.

The theory developed in this chapter represents a combination of the developments available in the literature. The textbooks used in this presentation of the theory in this chapter are listed below in the order of decreasing pertinence to this chapter.

Gould (G-3)

Bennett and Myers	(B-1)
Van Winkle	(V-1)
Holland	(H-2),(H-7)

Some of the other textbooks which present the basic principles of distillation are: (T-1), (S-1), (H-1), (C-1), (R-17), (C-5), (H-6), (H-5), (R-21), and (M-2).

II.1 DEFINITION OF BINARY DISTILLATION AND RELATIVE VOLATILITY

Binary distillation is defined as a process which separates a mixture of two components by utilizing mass transfer between the liquid and vapor phases of the components. The essence of this separation lies in the fact that when the vapor and liquid phases of a binary mixture are in equilibrium, the vapor is richer in the lighter component than is the liquid. The process by which the vapor phase becomes richer in the component which boils at the lower temperature (lighter component) is called mass transfer. Although the term distillation is occasionally used to describe the removal of volatile materials from solids, the term as used in this thesis will apply only to the separation of volatile components found in liquid solutions.

The equilibrium mentioned above is a phase equilibrium in which the properties of the two phases depend upon the physical characteristics of the two components which are present. The primary physical characteristic of interest in this thesis is the relative volatility α. If the concentration of the lighter component in the liquid phase is defined as u and the concentration of the lighter component in the vapor phase is defined as f(u), then the relative volatility is given by equation II.1. This expression is only valid when α does not vary

$$\alpha = \frac{1-u}{u} \cdot \frac{f(u)}{1-f(u)} \qquad \text{II.1}$$

with composition, which is a valid approximation for a large number of liquids. Equation II.1, then, defines equilibrium between the two phases in terms of the constant relative volatility α.

II.2 THE EQUILIBRIUM CURVE

The assumption that α is constant is essential to the developments of this thesis because it allows a specific equilibrium function to represent the characteristics of the phase mixture. Thus, an equilibrium phase diagram can be drawn as in Figure II.1 and a specific equilibrium function f(u) can be expressed in Equation II.2.

$$f(u) = \frac{\alpha u}{1 + (\alpha-1)u} \qquad \text{II.2}$$

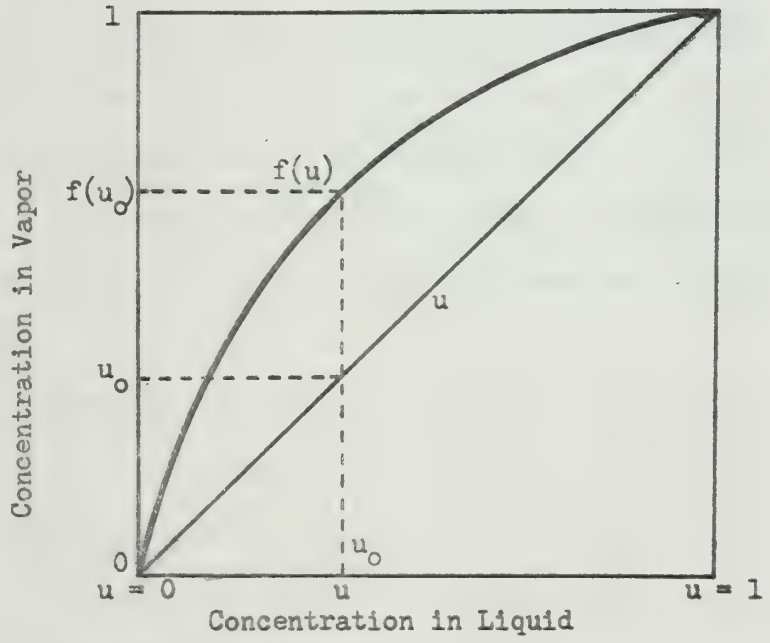


Figure II.1 - THE EQUILIBRIUM CURVE

In Figure II.1 the curved line (equilibrium curve) represents a graphical plot of equation II.2. If the relative volatility is not assumed to be constant, then this curve may have a significantly different shape and be represented by a different functional relationship. In trying to understand the meaning of the equilibrium curve it is helpful to consider a point u_o in Figure II.1.

Given a binary mixture which has liquid and vapor phases at equilibrium, then the concentration of the lighter component in the liquid is given by u_o, and the concentration of the lighter component in the vapor is given by $f(u_o)$. Thus, going from the liquid to the vapor in the two phase mixture corresponds to going from the u line to the f(u) line on the equilibrium curve. The fact that the relative volatility is such that $f(u) > u$ in this case implies that a partial separation of the mixture can be accomplished by separating the vapor from the liquid.

II.3 USING THE EQUILIBRIUM CURVE TO DESCRIBE SEPARATION

If the vapor is separated from the liquid in a two phase binary mixture, then condensing the vapor produces two separate liquids of different compositions, the one having been condensed being richer in the lighter component. This method of separation is the key to binary distillation.

This separation method can be visualized by using the equilibrium curve in Figure II.2. The original liquid at composition u_o is boiled and part of it becomes vapor at composition $f(u_o)$. If the vapor at $f(u_o)$ is then separated from the liquid at u_o and then condensed, the liquid condensate is of composition $u_1 = f(u_o)$. The new liquid at

composition u_1 can now be boiled to produce vapor of composition $f(u_1)$, where $f(u_1) > u_1$. Thus, by successively boiling and condensing the liquids and vapors, a desired degree of separation in terms of the upper and lower (on the graph of Figure I1.2) liquids can be achieved.

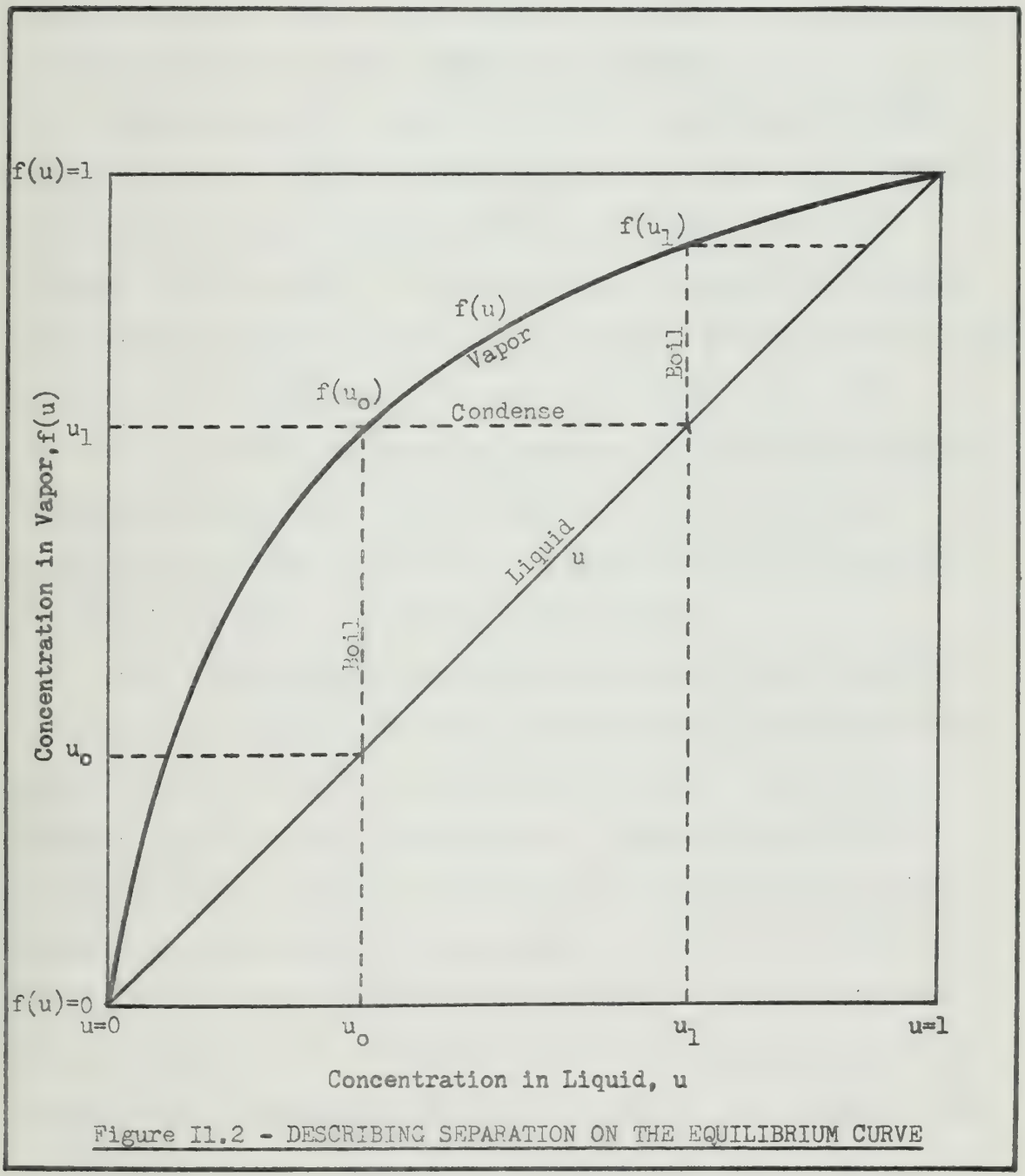


Figure I1.2 - DESCRIBING SEPARATION ON THE EQUILIBRIUM CURVE

II.4 PHYSICAL SEPARATION OF VAPOR AND LIQUID

The next problem to be considered is that of the physical equipment necessary to separate the vapor of $f(u_o)$ from the liquid at u_o, while at the same time allowing the liquid-vapor contact between the vapor at $f(u_o)$ and the liquid at u_1. There are two commonly used types of equipment for accomplishing this: packed columns and plate columns, both of which have innumerable variations.

Packed columns use a form of continuous contacting of liquid and vapor phases. This is accomplished by use of many small devices in the form of rings, saddles, spheres, etc., which are randomly "packed" into the column. This arrangement is designed to provide a very large surface area for a given tower volume because the contacting and mass transfer occur at the surfaces of the particles. The mathematical models (Section M) of packed columns are usually partial-differential equations. Packed columns will not be investigated specifically in this thesis, but it is expected that the developments of this thesis could be applied to packed columns.

Plate columns accomplish vapor-liquid separation and vapor-liquid contacting by allowing the liquid at composition u_1 to flow over the top of a plate, which is designed to let the vapor at $f(u_o)$ pass through into the liquid flowing over it. There are a multitude of different plate designs which accomplish this efficiently, such as bubble-cap, perforated, and sieve plates. Figure II.3 shows the basic physical characteristics of a bubble-cap plate. The concentrations shown in Figure II.3 correspond to those on the equilibrium curve of Figure II.2. Using these two figures one can see both physically and

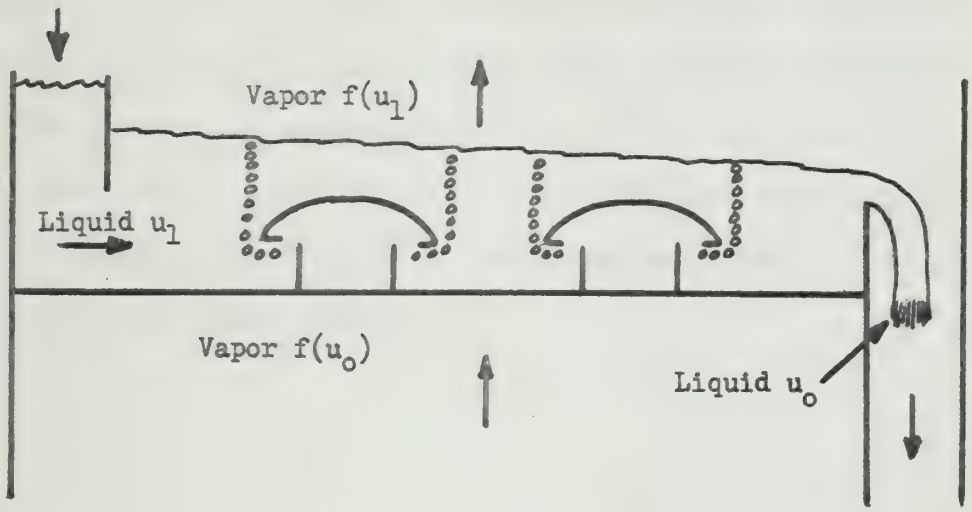


Figure II.3 - OPERATION OF A BUBBLE-CAP PLATE

conceptually how separation is achieved.

Physically, the liquid at u_1 enters the plate of Figure II.3 from the left-side downcomer of the plate above. The u_1 liquid then flows across the plate, in this case left to right, and is mixed (contacted) with the vapor $f(u_o)$ coming from beneath the plate. These two phases reach an equilibrium such that the liquid leaving the plate is at u_o and the vapor leaving the liquid is at $f(u_1)$. Since $f(u_1) > u_1$, a partial separation of the components results. Conceptually, following these same arguments on the lines in Figure II.2 reveals the properties of the mechanism of separation in terms of the mathematical expressions

describing equilibrium.

This chapter has presented the basic principles of binary separation using distillation. This separation has been described conceptually in terms of the relative volatility and the resulting equilibrium curve and physically in terms of the operation of a bubble-cap plate. The next chapter puts several of these plates together and presents the physical and conceptual descriptions of a complete distillation column.

CHAPTER I2

THE BINARY PLATE DISTILLATION COLUMN

The particular binary separation device chosen for study in this thesis is the plate distillation column. A plate distillation column is a vertical cascaded arrangement of individual plates (Figure I1.3) supported in a tower or column. The distillation column alone cannot perform separation but requires auxiliary equipment for its operation. This chapter presents a very brief description of the physical operation of a distillation column and its auxiliary equipment, a graphical description of its operation in terms of the McCabe-Thiele diagram, and a steady-state mathematical model of its operation.

I2.1 PHYSICAL OPERATION OF A BINARY PLATE DISTILLATION COLUMN

The physical separation of a binary mixture by an individual plate was described in Chapter I1. In general, one plate is usually inadequate to achieve the desired degree of separation of the mixture, thus many plates are combined in cascade to achieve greater output purity. An arrangement of eleven such plates is shown in the column of Figure I2.1. On any given plate in this column the liquid and vapor mix and reach equilibrium, with the vapor rising in the column plate-by-plate through the bubble caps and with the liquid flowing back and forth down the column.

Two of the auxiliary equipments necessary to the operation of the column are the condenser and the reboiler. The vapor flowing out of the top of the column enters the condenser where it is liquified and the resulting liquid is partially fed back to the top tray and partially removed as tops product. Similarly, the liquid flowing out the bottom

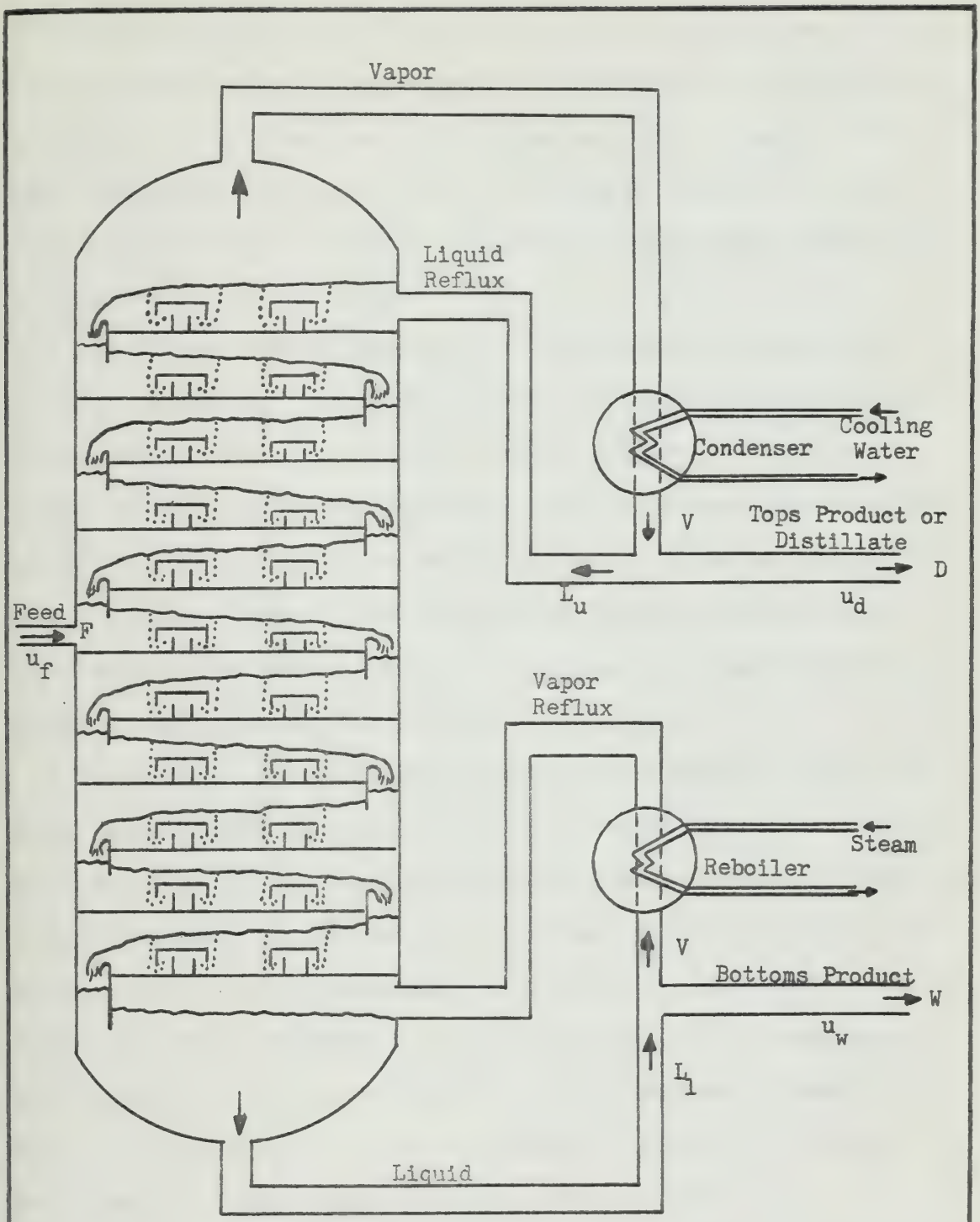


Figure I2.1 - A BINARY PLATE DISTILLATION COLUMN

of the column is divided into that portion removed as bottoms product and that portion which is vaporized in the reboiler and fed back to the bottom plate. The other auxiliary equipments, such as pumps to circulate the fluid, valves for control, structural supports, and many others, are not shown in Figure I2.1 but are, nevertheless, essential to the operation of the system.

Having described the operation of the internal cycling of the fluids in the column, the overall operation of the system can now be discussed. The input mixture to be separated is fed to that tray designated as the feed tray and enters the fluid cycle. The separated outputs are then taken off as the top and bottom products. Energy for operation of the system is supplied by the reboiler, steam heated in the case of the column of Figure I2.1, and energy is removed from the system by the condenser, water cooled in Figure I2.1.

There are innumerable types, arrangements, designs, and sizes of distillation columns, just as there are many different aspects of any given column which can be studied, such as chemical, thermal, structural, fluidic, economic, and environmental aspects. The central purpose of any column is to separate a binary mixture and the main criterion of "goodness" of the operation of the column is how well it performs this separation. Distillation columns are usually designed to separate the mixture to desired purity in such a way as to maximize the economic profit derived from the sale of the separated products.

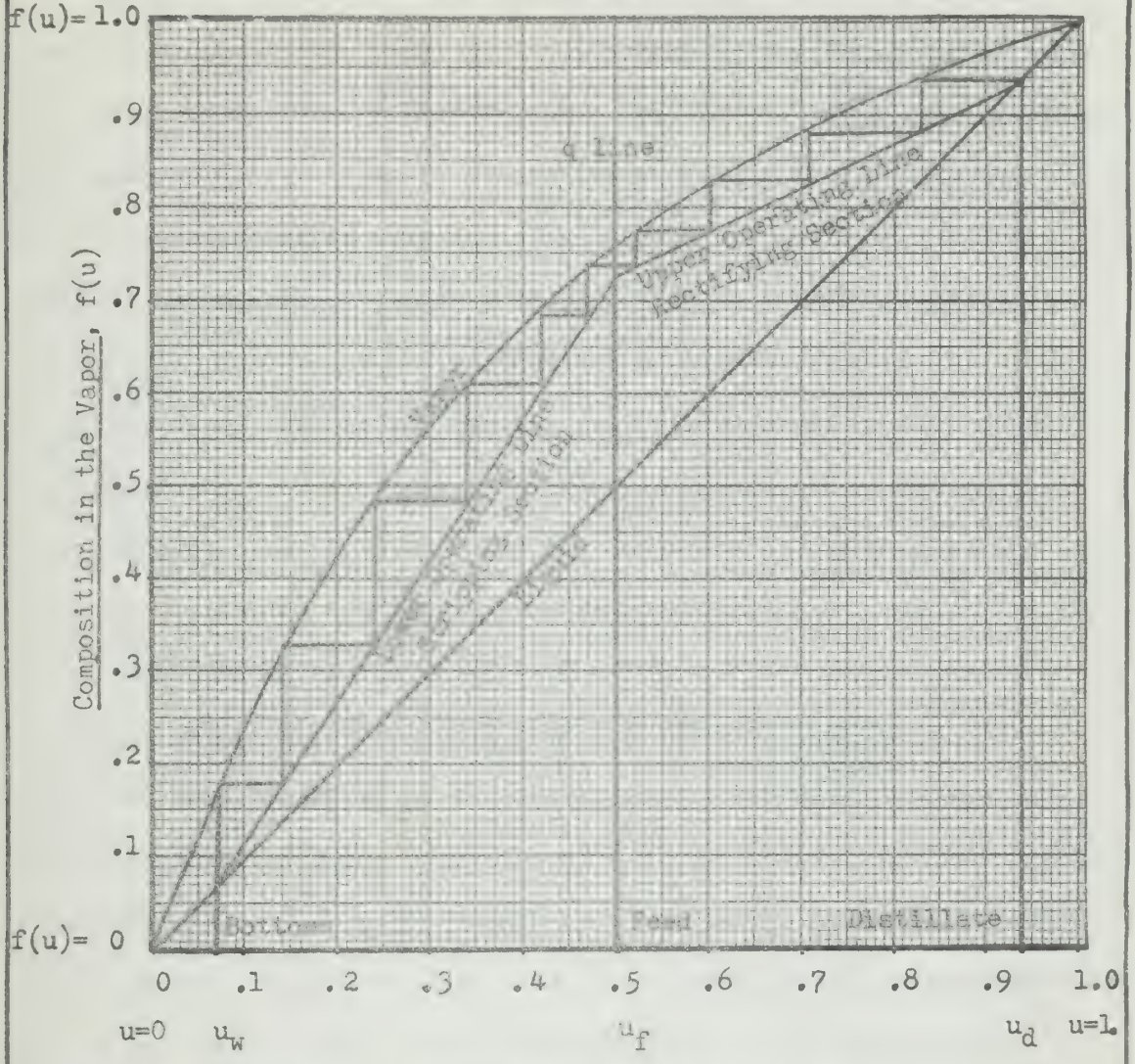
Output variations in the product purity greatly affect the profits derived from such sales. If the output is overly pure, then the revenue resulting from the sale of material thought to be of lower purity will

not be as high as it could have been. If the output is lower than the desired composition, then it cannot be sold at the price set for material of higher quality and profits will be reduced. Thus, composition variations in distillation column inputs and outputs are rather important, and mathematical models for the interaction between feed composition changes and output composition changes will be developed in this thesis for the purpose of studying such variations.

I2.2 THE MCCABE-THIELE DIAGRAM

One of the best graphical techniques for describing the steady-state operation of a binary plate column is the McCabe-Thiele diagram (M-10). A technique for describing the steady-state operation of the column is important to considerations involving variations in compositions, especially when composition variations are to be interpreted as upsets or deviations from an initial steady state to a final steady state. The basis of the McCabe-Thiele diagram is the equilibrium curve presented in Figure I1.2 for the operation of one plate. For the eleven (11) plate column of Figure I2.1 the McCabe-Thiele diagram for $\alpha = 3.0$ (M-15) is shown in Figure I2.2.

The graphical expression of the individual plate compositions presented by the McCabe-Thiele diagram gives both a qualitative and a quantitative view of the steady-state operation of the column. Qualitatively, it shows how the individual plates act to increase the purities of the output streams by operating in cascade with each step up the diagram representing a plate corresponding to a step up the actual column. Quantitatively, the individual plate steady-state compositions and the operating line slopes can be read directly from the diagram.



Operating Conditions

Plates = 11
L_u/V = 0.492
L_l/V = 1.522
u_f = .500
u_w = .068
u_d = .944
q = 1.0

Equilibrium Curve

$$f(u) = \frac{\alpha u}{1+(\alpha-1)u}$$

α = 3.0

Figure I2.2
MCCABE-THIELE DIAGRAM FOR
AN ELEVEN PLATE COLUMN (M-15)

The actual operating characteristics of the column are evident from the McCabe-Thiele Diagram. The amounts or percentages of liquid and vapor reflux flows determine the slopes of the two operating lines, the upper and lower lines in Figure I2.2. Each point of intersection on the operating lines represents the liquid composition of a plate, and thus the number of liquid points equals the number of plates in the column. Each point of intersection on the equilibrium curve represents the vapor composition between two of the column plates. The intersection of the two operating lines is determined by the q-line which depends upon the properties and condition of the feed at u_f. All of these properties are represented by quantities and equations in the steady-state model of the distillation column.

I2.3 A STEADY-STATE MODEL OF A BINARY PLATE DISTILLATION COLUMN

This subsection begins the developments leading to mathematical equations describing the operation of a binary plate distillation column. A mathematical model of the steady-state operation is to be presented and explained. Since most of the detailed developments of steady-state models are well covered in the literature(See B2.1 - Steady-State Analysis and McCabe-Thiele Diagrams), the discrete-plate steady-state model and its symbols will merely be presented, not derived in detail, in this section. The format of this presentation will be to present the description of the symbols to be used, present the model, and give a brief explanation of the model and the assumptions behind it.

The presentation of the discrete-plate steady-state model begins by listing and describing the mathematical symbols to be used in the model. This list of symbols is found in Table I2.1. The symbols are

$$E_n = \frac{f'(u_n) - u_n}{f(u_n) - u_n} \qquad \text{I2.1}$$

Where $f'(u_n)$ is a non-equilibrium state

u	Concentration of the lighter component in the liquid (lbm mole lighter comp./lbm liquid)
$f(u)$	Concentration of the lighter component in the vapor (lbm mole lighter comp./lbm vapor)
α	Relative volatility (dimensionless); assumed constant
F	Feed rate (lbm liquid/hour)
D	Distillate rate (lbm liquid/hour)
W	Withdrawal rate of Bottoms Product (lbm liquid/hour)
L_u	Liquid rate in the upper section (lbm liquid/hour); assumed constant
L_l	Liquid rate in the lower section (lbm liquid/hour); assumed constant
V	Vapor rate in the column (lbm vapor/hour); assumed constant
B_u	Upper reflux ratio (lbm liquid/lbm vapor), L_u/V
B_l	Lower reflux ratio (lbm liquid/lbm vapor), L_l/V
k	Feed plate index (number); integer
n	Internal plate index (number); integer $1 \leq n \leq N$
q	Portion of the feed which adds to the lower liquid rate; $L_l = L_u + qF$

Table I2.1 - LIST OF SYMBOLS USED IN DISTILLATION COLUMN STEADY-STATE MODELS

fairly standard throughout the literature with one important exception. Usually, in the literature, the composition of the lighter component in the liquid is represented by x and that in the vapor by y. In this thesis x will be used in Sections M and L to represent a continuous-spatial variable or continuous-plate-number variable; and y is not used, but the term f(u) is used instead. The term f(u) is standard in most of the literature. The symbols in Table I2.1 also apply to the corresponding symbols placed on Figure I2.1.

Figure I2.3 presents the discrete-plate steady-state model of a binary plate distillation column. This model is merely a combination of the conservation-of-mass equations (Inflow = Outflow) for each plate and a listing of the end, feed, and equilibrium description. These equations say mathematically what the McCabe-Thiele diagram says graphically. Solving these equations mathematically for the plate compositions is also equivalent to "stepping off" the compositions on the McCabe-Thiele diagram. The amount of mathematical manipulation involved in solving for the plate compositions when there are many trays is rather large when compared with the ease of stepping off these numbers on the McCabe-Thiele diagram.

Several very significant assumptions are implicit in the model statement of Figure I2.3. The upper and lower liquid rates, the column vapor rate, and the relative volatility have all been assumed to remain constant. In addition, the Murphree (M-8) efficiencies E_n defined in equation I2.1 have all been assumed to be unity, or equivalently, the assumption is made that each plate operates at complete equilibrium.

Model Equations

Rectification Section (Upper)

$$f(u_{n-1}) = B_u u_n + (1-B_u)u_d \qquad k+1 \leq n \leq N$$

Stripping Section (Lower)

$$f(u_{n-1}) = B_l u_n + (1-B_l)u_w \qquad 1 \leq n \leq k$$

Where $B_u = L_u/V$ and $B_l = L_l/V$

Equilibrium

$$f(u_n) = \frac{\alpha u_n}{1+(\alpha-1)u_n}$$

End Conditions

$f(u_N) = u_d$	Top	$n = N$
$u_k = u_f$	Feed	$n = k$, $q = 1$
$u_1 = u_w$	Bottom	$n = 1$

Feed Condition

$L_l = L_u + qF$ or $B_l = B_u + qF/V$; $q = 1$ in this case.

Figure I2.3 - DISCRETE-PLATE STEADY-STATE MODEL

To summarize briefly, Chapters I1 and I2 present the basic principles and mathematical descriptions for the operation of a binary plate distillation column. This presentation takes the form of a graphical description in terms of equilibrium curves and the McCabe-Thiele diagram, a brief physical description, and a set of mathematical equations forming a discrete-plate model for the steady-state operation.

The mathematical developments of this thesis in terms of distillation column dynamics or transient models continues in Section M. In that section, the discrete-plate steady-state model in Figure I2.3 is seen to be a subcase of the discrete-plate dynamic model, and a continuous-spatial steady-state model (not presented) is seen to be a subcase of a continuous-spatial dynamic model.

CHAPTER I3

PHILOSOPHY AND DISTILLATION

This chapter is purely opinion and will be written using the first person. It seems to me that some comments can be made about two very general philosophical desires as applied to the process of distillation. The first of these is the desire to observe and explain reality and the second is the desire to achieve profit. Philosophy is the study of the principles of reality, and distillation is a process for separating components; these two would seem to be almost completely unrelated, but, on the contrary, I think a definite and crucial relationship exists and propose to present it in this chapter.

I3.1 EXISTENCE EXISTS!

The fundamental axiom of reality is that existence exists, or as Aristotle stated, "A is A" (B-28). I exist in this reality as a being of volitional consciousness with only two choices open to me: to live or to die. I choose to live. I cannot live except by acquiring knowledge of one form or another. My only means of acquiring knowledge is through my senses. The only tool which I have for the thinking required to acquire knowledge from the inputs of my senses is the ability to reason. Reason requires the use of logic which is "the art of non-contradictory identification" (Atlas Shrugged - Ayn Rand). Thus, I wish to acquire knowledge about reality by observing it and applying logic to those observations.

One of the many questions I might ask is, "Does there exist a defined limit to the amount of knowledge attainable from the observations

of my senses and any devices which I may design to aid them?" If I wish to observe the operation of a distillation column, can I say beforehand that I'll never be able to understand completely the exact mechanisms or motions undergone to achieve the desired separation of components? I think that there are several practical resaons why the answers to these questions for an individual must be YES, even though the philosophical axiom A = A implies that the answers must be NO.

The first practical constraint that I run into is my limited physical capacity for knowledge in terms of my limited lifetime for acquiring it. But suppose for a moment that I am granted an infinite lifespan in which to observe and apply logic to distillation columns. I might then attempt to make more specific models of the column based upon more accurate observations of its operation. At some point, however, I run into another practical constraint: my act of observing the operation of the column begins to affect the operation which I'm trying to understand. This would be some form of "uncertainty principle" applied to distillation column measurements.

Suppose I don't accept uncertainty; after all, I'm certain that A = A. This supposition means that I can eventually determine a model of the operation of a distillation column that tells me to $N \rightarrow \infty$ decimal places exactly what each molecule, atom, or even sub-atomic particle is doing within the column at any time, including the effects of my observations. Thus, philosophically, the axiom A = A implies that unlimited reason is competent to define reality.

The certainty of limited life spans of individuals imposes a practical constraint on the amount of knowledge about distillation attainable by any one man. The assumption that human life will propagate forever through time implies that unlimited reason exists. Accepting this assumption one can say that man, now and future, has the unlimited reason necessary to define reality. What, then, determines the portion of the limited facilities of an individual which will be applied to the study of distillation? This, then, gets into the area of the second philosophical desire, or necessity: to achieve profit in order to live.

I3.2 INDIVIDUAL PROFIT MAXIMIZATION

The amount of effort devoted by any person to the study of distillation will be in proportion to the benefit (or profit) returned to that individual as a result of his efforts. For some this benefit may be derived by placing high value upon the self-satisfaction of explaining, even partially, the operation of a complex physical system, i.e. knowledge for the value of knowledge. Knowledge contains no life sustinence, and one who places a very large personal value in knowledge must have other means of attaining that profit convertible to life sustinence, either by selling that knowledge for food or by devoting a portion of his efforts, which could have been spent on studying distillation, to the acquisition of food by some other endeavor.

It is my opinion that each individual attempts to maximize the value to him (profit) of the use of his intellect. The individual who receives a small (but adequate for life support) income and devotes the remainder of his life to watching television is maximizing his

value implicitly by placing high value on the endeavor of watching television. However, in order for such an individual to have received that income necessary for life support, he must have devoted energies to some endeavor in which the profits are transformable into food. Thus, the conclusion can be made that no matter how an individual seeks to maximize the returns from his endeavors some portion of his life must be devoted to endeavors which produce something which can be transformed into food.

The question of whether or not there will definitely be people throughout time who will devote a portion of their life to studying distillation then becomes equivalent to asking whether or not distillation is an endeavor which produces something which can be transformed into food. If distillation is a profitable endeavor, then the relative question of how much of an individual's life will be spent studying it is answered by defining just how profitable distillation is to the man who studies it.

I3.3 PROFIT IN CERTAINTY

A distillation column has an input, which is a mixture of two components, and two outputs each of which, one is certain, contains a higher concentration of a given component of the mixture. It is a fact that in the present world the total value of the two outputs is greater than the sum of the mixture value and the value given up to perform the separation. Thus, distillation IS a profitable endeavor. WHY?

Distillation is profitable because certainty is of very high value. The operation of a distillation column produces two outputs

of greater certainty than the input. The fact that the composition of the outputs is certain is directly transformable into values equivalent to food and, as such, is a profitable endeavor for an individual to use for life support. The existence of profit from some endeavor implies that the benefits derived from it are greater than the costs incurred.

What is the cost of certainty? Suppose that I knew a microscopic man capable of distinguishing between the two different molecules of a binary mixture and capable of deflecting one type of molecule in one direction and the other type in another direction. My microscopic friend could then be the Maxwell's Demon of distillation if I let him stand in the inlet of the feed pipe to the distillation column and bat the lighter molecules upward and let the heavier ones fall, separating the mixture for me. I could then shut down the reboiler and condenser and sell the resulting pure outputs with no cost to me in terms of energy supplied to the distillation column. In fact, I could reason that the only effort involved in the entire process is the intellectual effort exerted by my small friend in recognizing which molecules are which. Thus, the cost of certainty is the information supplied by my friend.

A supposed fallacy of this argument is often presented as follows. The second law of thermodynamics states that entropy is always increasing in a real, physical process; entropy is then equated to average uncertainty, and uncertainty is defined as loss of information. So, somewhere down the line, someone loses out; in this case it was, according to this argument, my small friend. The Demon's information

was being transformed into my profit. The cost of certainty is increased uncertainty, if one accepts the concept of average uncertainty.

Suppose, once again, that I state that my concept of existence denies uncertainty the right to exist for all time. The concept NOT is the negation of reality and, as such, cannot exist. No-one will ever observe the color Not-Blue because it cannot exist as such. The use of the concept of average uncertainty is a denial of the statement A = A and can only be rejected as false if A = A is accepted as true. The average uncertainty argument implies that uncertainty is always increasing; A = A implies that certainty is increasing. The two are diametrically opposed. I accept A = A and deny that the universe is running down.

What then is the cost of the separation achieved by my small friend if I reject the concept of average uncertainty? The cost is the certainty used by my friend in separating the mixture. The profit which I derive from the sale of the two separated components results from the fact that the two separated components have greater certainty and therefore greater value than the value of the certainty used by my friend in separating the mixture. Thus, I can pay my friend for his services and we'll both be better off as a result of the process. Thus, all profit is the result of certainty.

I3.4 CERTAINTY AND KNOWLEDGE

The only route to certainty is through knowledge. The only route to knowledge is through observation and reason utilizing logic. If I desire certainty about the operation of a distillation column, then

I must turn one on (or read about someone who did), watch it, and apply reason to my observations to acquire knowledge about it. My limited physical capacity and lifespan dictates that my optimum acquisition of knowledge about distillation occurs during the time span up to the point where my marginal acquisition of certainty for expenditure of concentration begins to become negative. Beyond that point I would be better off studying some other profitable venture. Thus, constraints must be imposed on the acquisition of knowledge about distillation.

The physical capacity constraints of an individual are realistically applied to the study of distillation through judicious approximation. I realize that given enough time and intellectual capacity I could explain distillation to any desired completeness. However, in order to acquire any knowledge about distillation to use in deriving profit from my study, without already understanding it completely, I must make simplifying approximations and build up a hierarchy of knowledge pertaining to the subject. This is exactly what is done, and the following sections in this thesis present a theory which overflows with simplifications and approximations. The final test of any theory based on approximations must be that the revenue resulting from application of the theory is greater than the expenditure of effort in developing it. Such a test has yet to be applied to the theories presented in this thesis.

I3.5 WHAT'D HE SAY?

This chapter has presented my opinions concerning the relationship between my concept of philosophy and the study of distillation.

The chapter begins with arguments which position me as a human being within the framework of reality as a being who must know to exist. The reason I must know is that I must acquire profit (food) to live. Distillation is shown to be profitable by arguments which show that distillation increases certainty (value) and by arguments which show that uncertainty cannot exist if one assumes that existence exists. The same arguments are used to invalidate the uncertainty principle and the concept of average uncertainty. Finally, the use of simplifications and approximations in the study of distillation is justified on the basis that a man has limited facilities for use in studying it.

CHAPTER I4

A BRIEF REVIEW OF THE LITERATURE OF DISTILLATION

The volume of literature available pertaining to the study of distillation is completely overwhelming! It is easy to see why there can be no "Renaissance Man" in modern times. The bibliography presented in Chapter B1 of this thesis contains 352 references of which 202 pertain to distillation column dynamics and control. The 352 references are minute in number compared to the total literature. The 202 references represent a significant percentage of the total material available pertaining to column dynamics and control. By far the greatest proportion of the total literature of distillation deals with column operation, design, and steady-state analysis.

Distillation is such a general area and has so many interactions with other areas that it is easy to see why so much can be said about it. The areas listed in Chapter B2 represent, in themselves, an extensive collection of knowledge, and the list is far from complete. In this thesis the term "literature" will refer to this infinitisimal subset of 352 references.

The purpose of this chapter is to present descriptions, comments, and notes pertaining to some of the references in Chapter B1. With the exception of some of the theses, each entry in the bibliography was very cursorily inspected by the author, and some notes and comments were made where deemed worthwhile. This chapter is a connected listing of those notes presented in the format of Table B2.1. No attempt has been made to list complete descriptions, and the author

has chosen to use abbreviated language (incomplete sentences, minimum articles, etc.) to increase the densite of information with, hopefully, minimum loss of comprehension.

Many of these comments represent this author's opinions and should be evaluated as such by the reader. Those references in Chapter B2 under each area about which no information is given were most likely:

a. Dynamic response or control theses not read (not available)
b. Poorly written or invalid (author's opinion)
c. Not understood by the author after reading, but seemingly applicable
d. Those presenting material covered better in other references (author's opinion)
e. Partially explained by the title
f. Not really significant to the area but containing pertinent material
g. Discussed under another area in which case the area will be listed.

The last name of the first author of each reference is listed for the mnemonic convenience of the reader. In the interest of space conservation without loss of meaning all area titles and subtitles in Table B2.1 have been numbered and brought to the margin.

I4.1 GENERAL THEORY OF DISTILLATION

1. Textbooks

(B-1) Bennett & Meyers - covers heat, mass, momentum transfer, binary and multicomponent distillation, stagewise operations - primarily chemical engineering presentation; good presentation

of basic principles of distillation and steady-state analysis.

(G-3) Gould - very general process control text; presents detailed mathematical methods, models, and analysis for the dynamic behavior and control of a large number of chemical processes, including packed and plate columns.

(H-10) Henley & Staffin - very clear presentation of basic principles of distillation.

(R-23) Reid & Sherwood - presents in great detail the equilibrium, diffusion, thermodynamic, and thermal properties of liquids and gases.

(R-21) Robinson & Gilliland - detailed presentation of basic principles and steady-state analysis.

(V-2) Van Winkle - guide to fractional distillation design; considers hydraulics, multicomponent aspects, all sites of distillation design of plate and packed columns; discusses history of distillation; see also 3.

(A-19) Aris - steady-state distillation analysis.

(B-15) Bodman - presents Fortran IV program for optimum design of stagewise - ethylbenzene vacuum distillation reactor; economic optimization.

(M-14) McCabe & Smith - recent text presenting basic principles.

(O-2) Oliver - recent text presenting basic principles.

(H-2) Holland - uses Thiele-Geddes calculational procedure and θ method of convergence; mostly steady-state; "Instead of seeking exact analytical solutions for models that roughly approximate the actual system, researchers have put a vast amount of effort

into the development of iterative procedures in which progressively better initial values of the independent variables are selected for each successive trial."

(H-9) - 8.

(H-18) Hengstebeck - Considers many aspects of column design; presents basic principles and steady-state analysis; practical text.

(L-26) - 9.

(C-1) Campbell - steady-state analysis; dynamic analysis using signal flow graphs, frequency analysis; process control.

(P-3) Peters - plant design using detailed plate and bubble cap design equations; economics of distillation; optimum reflux design.

(P-10) Pratt - recent text presenting basic principles, steady-state analysis, and column design principles.

(R-22) - 6.

(R-17) Rosenbrock & Storey - extensive coverage of practical mathematical techniques for process dynamics.

(S-8) Shreve - large number of industrial processes described in detail, with diagrams and non-technical descriptions, very little mathematics; book represents a lifetime of experience in the chemical industry; chemical engineering = unit processes (chemical changes) + unit operations (physical changes).

(S-9) - 30.

(S-3) Sawistowski & Smith - steady-state analysis and calculation.

(S-1) - 30.

(T-1) Treybal - steady-state analysis and column design principles.

(B-12) Bird - mass transfer in terms of general conservation and diffusion equations; some transient analytical analysis.

(H-5) Henley & Bieber - steady-state example, 3 tray column, $\alpha = 2.5$, benzene - toluene.

(C-7) Chilton - cost analysis of distillation columns, y = cost $ installed per plate or foot, x = diameter squared, then the approximate equations for column cost are:

Plate Columns - stainless - $y = 6.47\ x^{0.63}$

Packed Columns - stainless - $y = 9.82\ x^{0.55}$;

distillation column maintenance 5-50 $/ft^3 bubble-plate, 3-10 $/ft^3 sieve plate, 5-15 $/ft^3 for packed columns per year in 1960 $.

(M-2) - 43.

(V-3) Vilbrandt & Dryden - steady-state design of columns; "In distillation columns, the pivot point in design is the reflux ratio (B_u in this thesis), which can vary between minimum and total reflux. Higher reflux ratios require greater quantities of steam and cooling water and a larger column diameter, but the column height requirements are lowered. The economic reflux ratio is usually 1.1 to 1.2 times the minimum for most cases."

2. Extensive Bibliographies and Literature Surveys

Literature Surveys from Industrial and Engineering Chemistry

Process Control

(W-16) (W-9) (W-15) (W-8) (W-19)

(W-10) (W-12) (R-25) (W-17) (F-6)

(W-11) (W-13) (W-18) (G-10) (W-23)

Distillation

(B-17) (B-18) (B-19) (F-8) (G-9) (F-7)

(R-12)-14.; (R-8)-21.; (H-7)-12.; (R-18)-16.; (H-8)-10.;

(R-17)-1.; (W-26)-41.; (Z-3)-19.

(G-14) Geddes - gives outline of developments that contribute to present knowledge of fractionator design in historical sequence; gives comments on present status and future problems; "If long-term funds were available for basic research on bubble plates, a substantial part of these should be assigned to scientific study of the fluid dynamics of plates."

References of Historical Interest

3. General Distillation

(L-19) Lewis - very early (1909) presentation of basic principles; uses equilibrium and phase diagrams.

(M-10) McCabe & Thiele - the most referenced paper in the literature; original (L(25)McCabe-Thiele graphical diagram of steady-state column behavior; all previous methods (Sorel's was the first in 1899) analytical; algorithm for stepping off tray concentrations on the equilibrium diagram.

(L-25) Lewis - early (1922) presentation of stagewise steady-state calculations.

(M-9) Murphree - explains McCabe-Thiele Diagram in equation form.

(V-2) Van Winkle - brief history of distillation - first recorded distillation in Egypt 50 BC, expect earliest unrecorded

distillation 2000 BC, fresh water distilled from sea water 300 AD, beverage alcohol process first industrial distillation process during 11-14th centuries, first books on distillation 16th century, stills were differential batch type with little reflux up until 19th century, 19th century began using steam (1800), bubble caps (1822), continuous still (1830), late 19th century first recorded mathematical discussions of distillation by Sorel (1899) and Hausbrand (1893), then 20th century began mathematics and improved distillation (L-19), (M-10), etc.

(U-1) Underwood - the best single presentation of the history of distillation in the literature, many pictures and diagrams of ancient methods.

(R-29) Rodebush - early (1922) plate-by-plate graphical technique; preceded McCabe-Thiele analysis.

(E-3) Egloff - review and diagrams of 15th-16th century distillation methods and apparatus.

(C-14) Cope - early (1932) graphical method using McCabe-Thiele stepping type design on the lower part of the equilibrium diagram.

(P-12) Peters - plate-by-plate calculations on the equilibrium diagram (1923) shortly after McCabe-Thiele.

(T-6) Thiele & Geddes - referenced many times in the literature, graphical and mathematical steady-state analysis and calculation method.

(G-14) - 2.

(I-1) IBM 705 Program - (1959) steady-state computer program to perform Thiele-Geddes calculations; one of the first industrial programs.

(A-17) Acrivos & Amundson - presents history, basic principles of distillation, steady-state analysis using numerical methods and eigenvalues.

4. Dynamic or Transient Analysis

(M-8) Murphree - (1925) first presentation in the literature of a discrete-plate dynamic equation; derives holdup equation, 1 ordinary differential equation, solves as an exponential.

(B-29) Berg & James - (1948) early column transient behavior considerations; mainly concerned with startup problem, early presentation of continuous-spatial model with partial differential equations, boundary conditions, and solutions, solves using linear equilibrium $f(u) = mu + b$, experimentally verified results.

(L-2) Lapidus & Amundson - (1950) early transient analysis; generalized the results of (M-1) for countercurrent absorption, showed how outlet concentrations could be predicted from the time course of the two inlet compositions, assumes $f(u) = mu + b$ equilibrium, uses Laplace transforms, poles & zeroes, linearized CSE, difference equations, entirely mathematical; calculates several transient responses.

(B-7) Bartky & Dempster - (1948) early solution to the transient system of plate equations, analogous to the classic start-up problem except that top reservoir has some holdup as individual stages, solution only approximate since compositions derived using $\alpha \approx 1.0$.

(R-2) Rose & Johnson - (1953) early development of binary system model; relative volatilities, total flow rates, and holdups independent of time, discrete-plate equations solved by Euler predictor method.

(R-12)-14.; (J-1)-21.; (F-5)-19.

5. Steady State Analysis and McCabe-Thiele Diagrams

(E-4) Eckhart & Rose - steady-state prediction, discrete-plate equations, linear equilibrium $f(u) = mu + b$.

(H-26) Hartland - analytical, steady-state comparison, boundary conditions.

(C-9) Cichelli - steady-state analysis, relates number of plates and reflux ratio to the sharpness of separation in binary batch distillation, graphs and equations for operation at any desired separation are given, many curves, sharpness of separation defined in terms of the "pole height," Rayleigh equation used.

(M-18) Mills - List of steady-state computer programs for equilibrium, enthalpy, etc., calculations.

(P-8) Prausnitz - steady-state computer subroutines for column calculations for bubble temperature, dew temperature, bubble pressure, and dew pressure.

(S-15) Surowiec - ideal cascade requires twice the minimum number of stages.

(S-20) Strand - good development of discrete-plate steady-state equations.

(Z-2) Zuiderweg - general steady-state comparison of device characteristics and plate efficiencies.

(F-3) Friday & Smith - discusses mathematically the formulation of a solution method for the equilibrium stage steady-state model; develops procedure for solving the concentration matrix equations which avoids truncation error build up, does not require mesh points, works equally well for any number of feeds and side streams, and handles nondistributed components.

(F-4) Furzer - nonuniform vapor distribution causes reduced efficiency, investigates plug flow model and perfectly mixed model, shows that maximum reduction in efficiency is halfway between these two models.

(H-30) Himmelblau - general, recent process mathematical modeling text, block diagrams, frequency analysis, matrix analysis.

(J-7) Jenson & Jeffreys - steady-state distillation analysis and mathematics, numerical methods for solving ordinary and partial differential equations, matrix methods, orthogonal function theory; primarily a mathematics text.

(L-12) Lowenstein - uses normal (Gaussian) probability distribution scaled graph paper to greatly increase the accuracy of the McCabe-Thiele diagram at the ends, i.e. at very high and very low separations.

(A-10) Amundson & Pontinen - discrete-plate numerical steady state calculations, uses cubic equilibrium relationship, quadratic expression for enthalpy, temperature distributions, 4-5 iterations on 15 plate column; results cited in (M-15).

(B-26) Barker - efficiency, design, experimental analysis of bubble-cap trays.

(S-12) Sargent - steady-state multicomponent column numerical technique and digital computer design; considers individual plate efficiencies and equilibrium curve; no dynamics.

(D-2) CEP Reprints - collection of steady-state distillation papers; articles covering heat and mass transfer, vapor-liquid equilibria, packed columns, tray column steady-state performance.

(R-30) Rose - experimental evaluation of column steady-state.

(S-24) Surowiec - steady-state column design using McCabe-Thiele diagrams and discrete-plate equations.

(S-23) Stanislas - general steady-state characteristics; plate efficiencies, equilibrium, etc.

(S-29) Sujata - plate-by-plate, steady-state calculations.

(F-9) Floyd - locating feed trays for lowest cost operation, steady-state.

(E-1) Edmister - true boiling point (TBP) defines distillation curve, distillation curve considered continuous and steady-state solved by graphical integration technique.

(T-7) Treybal - graphical technique for finding plate efficiencies based upon McCabe-Thiele diagram, operating lines and equilibrium curve.

(S-16) Srygley - optimum steady-state design in the sense of minimum number of plates for desired product purity; uses Thiele-Geddes θ-method of convergence, sequential search for optimum.

(B-1)-1.; (M-10)-3.; (H-10)-1.; (H-18)-1.; (M-8)-4.; (M-9)-3.; (B-10)-30.; (C-1)-1.; (V-2)-1.; (G-3)-1.; (H-5)-1.; (H-2)-1.;

(A-17)-3.; (C-14)-3.; (O-2)-1.; (T-6)-3.; (R-5)-16.; (R-21)-1.; (T-1)-1.; (S-3)-1.; (H-21)-19.; (I-1)-3.; (L-25)-3.; (A-19)-1.; (P-12)-3.; (R-1)-16.; (R-29)-3.; (S-1)-30.; (S-7)-20.; (R-18)-16.

6. Structural Design

(L-13) Lowenstein - design of plate sizes using a nomograph and plate size "slide rule."

(R-22) Rose - minimum cost structural design considerations including wind loads, dead weight stresses, longitudinal stresses, thickness formulas, numerical examples, drawings of industrial columns.

(J-3) Jones & Van Winkle - experimental analysis of 3 inch perforated plate column to determine plate thickness effects on column properties.

(M-11) Manning - structural screens introduced to provide better mixing and increase column efficiency.

(L-12)-5.; (D-11)-16.

7. Economics and Operations Analysis.

(M-13) Mitten - economic optimization of distillation by dynamic programming.

(B-15)-1.; (S-8)-1.; (F-9)-5.; (C-7)-1.; (V-3)-1.

8. Thermodynamics

(H-9) Hougen - Covers, very extensively, thermodynamics applicable to distillation.

(R-23)-1.

9. Hydrodynamics or Fluid Mechanics

(F-4)-5.; (V-2)-1.; (B-12)-1.; (R-23)-1.

(L-26) Levich - analytical solutions to convection and diffusion equations including chemical aspects.

(H-14) Holm - concludes that vapor flow effects can sometimes cause Murphree efficiencies to be greater than unity.

(F-5)-19.; (T-7)-5.

(B-4) Bernard - considers sieve tray mixing, foam density, flow properties.

(S-19) Sakata - time for mixing, analytical equipment, mixing pools, plug models, and tray efficiencies.

10. Chemistry

(B-16) Black - simplified approach to phase equilibria, large number of phase equilibria for various compounds presented.

(H-8) Hala - extensive list of chemical compounds referenced to entries in a large bibliography; many phase diagrams presented,

(B-1)-1.; (H-10)-1.; (F-9)-5.; (T-6)-3.

(H-17) Harper & Moore - experimental paper showing a small still for measuring vapor - liquid equilibria lines, several lines given as examples.

(H-20) Howard - concludes that any unsteady-state distillation calculations should include plate, condenses, and reboiler holdups in order to include enough degrees of freedom.

11. Philosophy

(A-13) Aris - oftentimes engineer's rules of thumb are the only tools necessary to solve problems adequately, gives examples.

I4.2 DISTILLATION COLUMN DYNAMICS

12. Textbooks

(M-1) Marshall & Pigford - beginning of quantitative analysis of unsteady-state operation; many simplifying assumptions used to obtain analytical solutions using Laplace transforms, assumed equilibrium relationship $f(u) = mu + b$ with m, b depending only upon the identity of a component, assumed total flow rates and holdups independent of plate number and time; considers startup problem.

(H-7) Holland - uses numerical methods to solve process differential equations; uses θ-method for distillation discrete-plate equations, example step response of 3-tray column calculated; good literature survey; book emphasizes numerical methods and matrix methods.

(G-3)-1.

(F-16) Franks - modeling of chemical processes for the purpose of control, plate equations, partial differential equations.

13. Theses

(M-15) Mohr - considers each of two sections of a column independently, determines step response for each input stream using IBM 705 and discrete-plate equation, each of the response curves is then fitted with a two-time constant exponential expression, these expressions manipulated into general transfer function using Laplace transform variable p, time constants and gain factors of the column are then correlated with steady-state parameters from McCabe-Thiele diagram; analysis based on linear equilibrium $f(u) = mu + b$; assumes binary mixtures, constant α,

constant fluid rates, total condensation, negligible holdup, constant liquid holdup each plate, reboiler holdup equivalent to that on each plate, q = 1, perfect mixing, unity plate efficiencies; found that major time constant was independent of the type of disturbance, gains and secondary time constants vary with disturbance type and with initial steady-state, predicted responses of large columns more sensitive to changes in values of selection parameters than small columns; column time constants increase with H/L, degree of separation, degree of nonlinearity of equilibrium curve, number of plates.

(R-6) Romagnoli - hybrid simulation of discrete-plate equations; butadiene distillation plant, 2 towers of 49 trays each of bubble type, constant pressure, constant holdups, water ignored, vapor holdup ignored, constant Q, $E_n = 0.7$, Francis-weir formula, micro assembly language and PDP-1 used; conclusion was that hybrid setup worked faster than purely digital computation.

(B-32) Brosilow & Tanner - develops and analyzes methods for computing and optimizing countercurrent staged processes using distillation as an example; formulates models in terms of both discrete and continuous spatial equations; solves continuous models using economic cost criterion using gradient and Lagrangian non-linear programming methods; found equations much easier to solve when models were not restricted to integral values of stages, allowing more general optimization methods to be used such as Lees' method; two-point boundary

value problem solved by imbedding it into an initial value problem in time; found that when Lees' algorithm was modified to generate tridiagonal matrices the rate of convergence increased substantially.

(G-5) Gaydos - develops generalized digital computer program and model for a single bubble-cap plate; model includes multi-components, hydraulics, non-ideal vapor-liquid equilibrium, heat transfer to and from each stage, provisions for feed and take off streams; computation time limitations were encountered in the simulation.

14. Reviews, Bibliographies, and Literature Surveys

(A-3) Archer & Rothfus - presents survey of the 1955-1960 dynamic behavior literature; discrete-plate equations developed, startup and transition between steady states, batch operation of plate and packed columns, and process control are all discussed in terms of their respective literature; frequency analysis.

(R-12) Rosenbrock - surveys the history and present developments of discrete and continuous distillation and heat exchanges models; best presentation of this material in the literature.

(H-7)-12.; (R-8)-21.; (Z-3)-19.; (L-3)-15.; (T-2)-16.

(S-33) Lehigh Symposium - discrete-plate models, transient response, and control of distillation columns; extensive bibliography of 149 references on column steady-state, dynamic, and control aspects; frequency response analysis.

Additional surveys, see 2.

Dynamic Models or Solutions

Discrete Plate Equations

15. Frequency Analysis or Laplace Transform Solution

(A-3)-14.; (R-12)-14.; (H-7)-12.; (R-8)-21.

(Z-3)-19.; (S-33)-14.; (T-2)-16.

(L-3) Lamb, Pigford & Rippin - oscillations in tray compositions resulting from input oscillations in either feed composition or reflux flow are calculated using analog computer for 16-tray column; found frequency response at low frequencies like simple first-order process and at high frequencies having interference patterns and large phase lags; equations linearized about steady-state, E = 1, frequencies from 0.001 to 1 radian/tray holdup time, 5-tray column frequency response also obtained.

Transient or Time Analysis

Numerical Solution

16. Digital Computer

(D-4) Distefano, May, & Huckaba - (1967), discrete-plate dynamic model solved for a sequence of upsets in which the next step occurs before the transients of the previous one have died out; solves large system of equations by Adams-Moulton-Shell (AMOS) finite difference technique on IBM 709, computation time was 12 min., expect hybrid steup would speed this up, 12-plate column, spacing 1 ft, 10" diameter, samples of every 3rd plate, 7 runs for different types of steps and pulses; oriented toward prediction for feedforward control; transient times 40-80 min., experimental data agreed with computer

calculations to within 5%, error blamed on truncation in predictor-corrector methods.

(B-32)-13.; (R-4)-4.; (R-20)-31.

(D-8) Distefano - numerically solves discrete-plate equations by a large number of different methods and then compares them, (D-10) presents stability aspects.

(H-3) Huckaba - numerical solution by IBM 650 of transient response to binary 12-plate column, experimentally confirmed; uses nonlinear discrete-plate equations, inputs are step changes in heat input to the reboiler, feed composition, and simultaneous changes in feed composition and reflux ratio; computation time 5 min. using fourth-order Runge-Kutta for starting and fifth-order modified Adams for continuing.

(L-5) Luyben - uses set of linear perturbation type differential equations for characterizing dynamic behavior; experimental results verified for acetone-benzene system, $1.8 \leq \alpha \leq 2.2$; types of disturbances were changes in feed composition, feed rate, top tray reflux rate, bottom tray vapor rate, equations solved by analog computer.

(D-15) Duffin & Gamer - defines model for multicomponent distillation which includes secondary effects due to column hydraulics, holdup, and delay effects in boundary conditions; errors in generated system response at low values of elapsed time usually due to inadequate models; used general discrete-plate model and numerical integration scheme, conclude that model is valid.

(R-16) Rosenbrock - surveys available solution methods for the discrete-plate equations, decides to use digital computer for speed and generality; describes numerical method and program, computation time 5 min. for 5 plates up to 100 min. for 300 plates.

(R-9) Rosenbrock - develops discrete plate equations, discusses possible methods of solution, almost identical to (R-16).

(R-10) Rosenbrock - discusses relative advantages of two computer programs for solving the equations in (R-9); first program has f(u) fed in as table of 101 values, linear interpolation, forward integration used, first program finally rejected due to limitations; first program required solution of large system of simultaneous equations, second program developed to eliminate this by solving step-by-step by equating slopes; routine included to evaluate df(u)/du at discrete-points.

(R-11) Rosenbrock - discusses the accuracy of computer programs in (R-10), extends application to multicomponent systems; used equilibrium curve as $f(u) = u + 0.02$, $E = 1.0$; concludes that the most promising method for calculating transient response is digital computer.

(A-4)-40.; (R-17)-1.; (S-33)-14.; (S-16)-5.; (S-20)-5.

(M-3) Mah, Michaelson, & Sargent - dynamic behaviour of multistage systems described by large sets of non-linear first-order differential equations; discrete-plate equations then linearized but shown to be inconsistent due to linearization, step-by-step procedure using exponential function is proposed, numerical integration technique, reviews all standard numerical

procedures, uses tridiagonal matrix, finds eigenvalues, shows that use of linear equilibrium $f(u) = Ku$ also leads to physical inconsistency.

(T-2) Tetlow, Groves, & Holland - develops a generalized model which accounts for the effects of channeling, transfer lag, mixing, and mass transfer in unsteady-state, multicomponent, discrete-plate distillation; model tested on a large number of numerical examples; considers plug flow and perfect mixer holdups, large tridiagonal matrix results, θ-method of convergence used; use of the generalized model in the analysis of control systems is discussed.

(W-1) Wood & Armstrong - derives a linearized model of the discrete-plate equations using $f(u) = mu + b$ equilibrium; solves for step response of feed composition; comparison with experimental results shows that the model is only valid for moderate values of time after the step and cannot be used as the column approaches final steady state.

(P-2) Peiser & Grover - presents a model similar to (H-3) including the effects of heat and mass transfer and tray hydraulics; predicted that unsteady-state prediction can be used to solve several significant problems in multicomponent distillation which are not evident from steady-state analysis; numerical computations carried out on a digital computer simulating column open and closed loop control.

(D-9) Davison - solves large systems of $\dot{x} = Ax + Bu$ equations; calculates the poles and zeroes of the system, then solve for a few of the more significant variables in terms of poles and zeroes.

(L-18) Luyben - discrete-plate equations solved for transient response for use in feedforward control.

(D-6) Davison - discrete-plate equations solved using matrix methods for the transient response of a column due to pressure variations for use in control.

(S-6) Sargent - discrete-plate equations solved numerically using matrix methods.

(T-9) Thorogood - discrete-plate equations solved using Runge-Kutta methods.

(Y-1) Yesberg & Johnson - demonstrates use of a resistance network analog to solve the absorber problem of (A-1) and (L-2), discrete-plate equations linearized, time derivative represented by a backward finite difference to produce a set of simultaneous algebraic equations which are solved on an IBM 650 by matrix inversion.

(G-4) Greenstadt - discrete-plate equations solved by Newton's method.

(R-5) Rose, Sweeney & Schrodt - solves startup problem for ternary mixture using discrete-plate equations, Lewis-Matheson method used.

(D-11) DiLiddo & Walsh - pulse column considered as a series of stages, 3 plate ideal model, 9 plate real model, numerical solution on IBM 605.

(R-1) Rose, Johnson & Williams - (1950) discrete-plate equations solved by Euler predictor method; model assumes relative volatilities, flow rates, and holdups independent of time.

(R-19) Rose, Johnson & Williams - (1951) similar to (R-1), early papers showing pictures of IBM cards, plate equations solved by numerical methods.

(L-27) Lowe - discrete stage equations solved on digital computer, no distillation.

(W-4) Waggoner & Holland - discrete-plate equations solved using Simpson's rule, 3 point corrector to approximate the integrals in the component material balances, results presented in table form.

(R-18) Rose & Williams - (1950) early plate-by-plate solution of discrete model, similar to (R-19) (R-1), shows wiring of computer control panels.

17. Hybrid Computer

(F-1) Franks - solves several countercurrent problems, several of these were for distillation.

(F-13) Frank & Lapidus - discrete-plate equations solved by hybrid computer using one integrator for each plate.

(R-6)-13.;

(F-12) Frank & Lapidus - hybrid simulation particularly useful for nonlinear partial differential equations, uses repetitive analog operation, memory, and first-order lags.

18. Analog Computer

(B-23) Bowman & Clark - uses linear equilibrium f(u) = ku which was found to be valid near the top of the column where volatile component concentration is small, discrete equations for 20 and 30 plate columns wired up on analog computer; when column was switched from total reflux to finite reflux ratio, an almost instantaneous drop in overhead composition occurred, from this point on the overhead was independent of the time on total reflux and dependent only on the stillpot composition at the end of the total reflux period; this suggests that column can be divided into two independent sections, first would be period on total reflux, second would be behavior at finite reflux; linear equilibrium does not provide exact representation of real column, provides guide to the degree and direction of change within the column.

(P-1) Pigford, Tepe & Garrahan - solves unsteady-state equations for batch distillation of a binary mixture using a mechanical analog computer called the "differential analyzer"; assumes constant relative volatilities, vapor & liquid flow rates.

(R-3) Rose & Williams - demonstrated use of an analog computer to obtain transient response and design a controller for a 5-plate column, uses analog computer with Pade delay circuits; large number of problems solved to determine the best controller for maintaining the composition of the distillate constant under composition and thermal variations of the feed.

(G-12) Grover & Peiser - analog computer solves plate equations for control, stability aspects considered.

(L-5)-16.

19. Analytical Analysis

(D-3) Davidson - uses mechanical analog and Rayleigh's method to determine eigenvalues for finite series representation of plate column transient behavior; plate-type stripping column fed at top, no bottoms takeoff, assumes linear equilibrium; equilibrium concentration on any plate proportional to exp $(-\beta T)$, where β depends upon α and number of plates N; Rayleigh method used to give approximate β; solves example model of Taylor Diffusion type, found that first term in series was most important.

(G-2) Gilliland & Mohr - analytical analysis of discrete-plate equations using two-time constant exponential model of (M-15); digital computer solves for transient response, then the two time constants are determined from the results and used to develop transfer functions; by use of transfer functions, the responses of several columns to step changes in feed composition were predicted and compared with the responses calculated by numerically solving the discrete-plate equations.

(A-3)-14.; (M-8)-4.; (M-1)-12.; (R-8)-21.; (S-31)-43.

(R-7) Rosenbrock - funcamental "disturbance trapping" paper; characterizes the departures of a distillation column from its steady-state by a quantity D which measures the rates of change of composition on all the plates and increases whenever the column is disturbed from its steady-state; result is generalized

$$D = 2 \sum_{n} \left| d(H_n u_n)/dt \right|$$

to multicomponent systems; disturbances become "trapped: in the column at points where equilibrium curve slope equals operating line slope, rates of change of composition do not decrease as would be expected, numerical computation of behavior in these cases is difficult; presents an electrical analog to the discrete-plate equations.

(R-32) Rosenbrock - discrete-plate equations, matrix methods, energy considerations.

(W-2) Wilkinson & Armstrong - considered response of a column at total reflux to a change in bottom vapor composition, used binary mixture, linear equilibrium curve; response predicted by analytical analysis was in good agreement with that observed experimentally.

(F-16)-12.; (G-3)-1.; (H-20)-10.; (B-7)-4.; (B-12)-1.

(B-27) Balasubramanian - analytically solves one differential equation for a one-plate still.

(C-2) Cullinan - considers transient start-up problem using matrix methods for analytical solution, uses $f(u) = mu + b$.

(Z-3) Zykov - analytical solution of discrete-plate equations for transient analysis of multicomponent column; good bibliography of Russian literature.

(F-5) Foss, Gerster & Pigford - assumptions of complete mixing or no mixing lead to inaccuracies in distillation, paper attempts to establish the nature and extent of mixing and to develop calculational methods to account for its effect on plate efficiency; mixing experimentally determined by use of tracers and measurements of residence times; simplified calcu-

lation procedure presented which affords a rapid means of computing plate efficiency under all mixing conditions.

(H-21) Hassett - solves for transient behavior using equilibrium, steady-state, and McCabe-Thiele diagram.

Continuous Spatial Equations

20. Frequency Analysis or Laplace Transform Solution

(J-6) Jafri, Glinski & Wood - continuous system transient response with control using time constants and transfer function analysis.

(M-27) Majumdar - solves CSE using Laplace transforms and linearization, applies to Clusius column.

(H-4) Hoerner & Shiesser - frequency and time responses using Laplace transforms, linearized CSE, linear equilibrium; gives model of Taylor Diffusion type.

(S-7) Sellers & Augood - transients in a liquid hydrogen separator, uses Laplace transforms, exponential characterizations, rate of approach method.

(W-5) Ward - uses Laplace transforms and frequency analysis to calculate the time behavior of dynamical systems.

(D-1) Douglas & Rippin - uses linearized equations and sinusoidal inputs, considers system in terms of chemical oscillators.

21. Transient or Time Analysis

(J-1) Jackson & Pigford - (1956) digital computer solution of linearized CSE model for startup problem, plots of composition throughout column as a function of reduced time are presented; linearized CSE and linear equilibrium $f(u) = Au$ gives equation

of Taylor Diffusion model type; took 3 hours of computation time on IBM 701 to solve for transient curves on several trays.

(H-4)-20.; (D-3)-19.; (M-1)-12.; (C-2)-19.; (L-26)-9.

(K-2) Koppel - solves heat exchanger/chemical reactor equation of a form possibly similar to CSE;

$$\frac{\partial u}{\partial t} = [1 + r(t)] \frac{\partial u}{\partial x} + P[1 + br(t)] u^n \quad .$$

(O-1) Osborne - linear equilibrium f(u) = mu + b used, equations considered continuous in time and differenced in theoretical stage; concludes that the real cause of numerical instability problems is in theoretical stage direction differencing; numerical solution obtained with very large theoretical stage step, one theoretical stage, and very small time steps, this took care of instability problems; Fortran IV computer program for max. 6 components, max. 60 trays described.

(R-8) Rosenbrock - calculates transient responses; describes labor needed to solve CSE models; describes control aspects and theory; presents good bibliography.

(S-13) Stone & Brian - detailed numerical methods described for solving CSE type equations; solves Taylor Diffusion model equation as an example; CSE is a subcase of equation (2) which is a general form of convective transport equation;

$$\frac{\partial}{\partial x} [D(x,t,u) \frac{\partial u}{\partial x}] - \frac{\partial}{\partial x} [V(x,t,u)f(u)] = \frac{\partial u}{\partial t}$$

several different types of numerical methods discussed and compared; analysis derived applies only to linear equations;

recent results indicate that the desirable features of solutions obtained by the new equations for linear problems are to a large degree found in solutions of nonlinear problems.

(M-28) Montroll & Newell - exact solution of nonlinear differential equations which describe the time dependent behavior of multi-stage cascade separating processes of two very similar non-linear species, Rayleigh separation law postulated for each stage; linearization of nonlinear second-order portion differential equations is discussed; analytical expressions in terms of exponentials and eigenvalues are developed; equilibrium curve is approximated by $f(u) = u + cu(1 - u)$.

(K-3) Kermode & Stevens - several nonlinear continuous models solved on an analog computer.

(P-7) Powers - numerical solution to Taylor Diffusion type partial differential equation with two-point boundary conditions and one initial condition.

(R-14) Ruckenstein - analytical analysis of convective diffusion (Taylor Diffusion) type equations; extensive analysis of applicable transformations and linearization methods.

(B-29)-4.; (G-3)-1.

(T-5) Tsang - solves heat equation using eigenfunction expansion (orthogonal), evaluates 1st 3 values numerically; other analytical solutions presented also, Bessel functions.

(H-25) Herron & Van Rosenberg - uses a mesh and centered difference method to numerically solve convective transport equations with two-point boundary conditions.

(J-2) Jury - solves heat equation using analog computer, uses memory, solves repetitively.

(J-5) Jackson - numerical solution and optimization of partial differential equation models.

(L-20) Lapidus - transient response and control of chemical reactors using continuous models.

(B-20) Bedingfield & Drew - heat and mass transfer expressed by the same equations.

(W-14) Woodle - analogy between distillation and heat transfer, some equations.

(B-25) Brian - transient response using a continuous, Taylor Diffusion type model.

(C-8) Crank - diffusion in different geometrics with different boundary conditions, finite difference methods, diffusion and chemical reaction; use transformations for equations with variable diffusion coefficients.

Experimental Transient Behavior

22. Frequency Response

(H-15) Henley - frequency response techniques for experimental analysis of transient behavior.

(H-23) Hutchinson & Shelton - frequency response techniques using correlation functions.

(A-6) Armstrong & Wilkinson - carried out experimental work to verify theoretical computations and methods of (R-16) and (R-9); studied behavior of 21 plate CH_4 - CCl_4 separator subject to

step changes in feed and reflux on column composition; long time agreement was better than short time after disturbance; results summarized by transfer functions having the form of pure time delay followed by a linear log, both time constants are functions of plate number.

(H-24) Haagensen - experimental results derived from frequency response using matrix techniques.

(W-28) Woods - experimentally determined controller settings for a continuous system operating dynamically.

23. Time Response

(H-3)-16.; (L-5)-16.; (R-30)-5.

(B-5) Baber & Gerster - determines experimental transient response of column to changes in liquid and vapor rate, demonstrate the applicability of discrete-plate equations for predicting measured response; responses to step inputs presented in tables and graphs; equations solved by analog computer; results confirmed validity of model; linear perturbation types of equations predict satisfactorily the transient behavior.

(B-3) Baber - similar to (B-5) but earlier; experimental response of 5-tray, 2 ft. bubble-cap column; tests made over a range of gas and liquid rates nearly up to the flooding point and for tower pressures up to 5 atmospheres; average difference between predicted and experimental results was 13%, indicating that simple perturbation equations are valid models.

(R-15) Rademaker - tested an ethylene-ethane splitting column to provide data for checking a general theory of column dynamics;

data summarized in graphs and experimental accuracy discussed.

(D-12) Davies - "hidden transients" can have significant effects on tray efficiencies.

24. Cyclic Distillation

(A-14) Atkeson - one of the first papers (1957) to indicate that cycling or nonequilibrium operation can increase mass transfer rate greatly; attempts to explain physically.

B2.3 DISTILLATION COLUMN CONTROL

25. Textbooks

(A-12)-40.; (G-3)-1.;(C-1)-1.

(B-13) Buckley - very practical, industrially oriented process control text.

(K-5) Koppel - matrix theory, optimal control, sampled-data control.

(A-11) Athans & Falb - mathematical theory of optimal control; many examples and problems; very clear presentation; extensive bibliography.

26. Theses

(B-2) Beecher - presents method of dynamic control system synthesis using calculus of variations; provides extensive Fortran program; example is 100 plate butadiene/butiene-2 column.

(B-32)-13.

(G-1) Gordon-Clark - uses matrix theory to adjust dynamic response of process to some required response before applying conventional control; uses linearized model of a 5-plate binary column, control and measure composition on each plate; main computation difficulty is finding eigenvalues of matrix;

Fortran program, form matrix, form into tridiagonal matrix, obtain complex roots of real polynomial by Bairstowe's method, iteration using quadratic factor, obtain roots of quadratic factors, return; major drawback is large number of variables required.

27. Extensive Bibliographies and Literature Surveys

(A-3)-14.; (R-8)-21.; (R-12)-14.; (S-33)-14.

Conventional Control Systems

28. Digital Control

(H-29) Hanson, Duffin & Somerville - provides extensive Fortran computer programs for control.

(B-6) Buster - closed loop control applied to oil fractionating system, required large memory and clever programming to complete calculations in real time.

29. Hybrid Control

see 17.

30. Analog Control and Instrumentation

(H-16) Haines - large number of diagrams of possible column control configurations with explanations.

(G-3)-1.; (B-13)-25.; (C-1)-1.; (G-12)-18.

(B-22) Buckley - basic column control strategy, diagrams of control loops, linearized models.

(B-10) Bauer & Orr - uses McCabe-Thiele diagram to derive best operating lines for control.

(B-31) Boyd - mostly nonmathematical and non-diagramatical discussion.

(P-6) Pink - describes control using analog computer, no mathematics.

(S-1) Shinsky - process controls based upon time response analysis; distillation columns hard to control because (1) many trayed towers slow to respond to control action, (2) separation requires many variables, (3) on-line analysis not always available, (4) distillation units are usually last in the chain of processing operations, and (5) factors affecting separation not readily interpreted in terms of control system requirements.

(L-4) Lupfer & Parsons - describes a control system designed to reduce the effects of changes in flow rate and feed composition on column operation, uses predictive or feedforward control, dependent outputs of the process are controlled by measuring one or more inputs (which generally cannot be controlled), and then the controlled parameters are changed as required to achieve the desired output.

(C-12) Ceaglske - comparison of transient and frequency response methods for control of linear chemical process systems.

(T-11) Tivy - control discussion, no mathematics.

(M-29) Moczek - discusses effect of transient behavior and dead time on control, very little mathematics.

(P-14) Phillips - control descriptions, no mathematics.

(R-13) Rijnsdorp - discusses feedforward & feedback control with distillation column as an example.

(S-9) Strobel - describes in detail theory of optical and electrical measuring devices; great deal of theory presented, photometers, spectral analysis, wave theory, etc.

(H-1) Harriott - transient and frequency analysis used for column control.

Control Systems Using Dynamic Models

31. Digital Computer Control

(A-12)-40.; (D-4)-16.; (L-18)-16.; (D-6)-16.

(R-20) Rosenbrock - application of automatic control theory to chemical processes has not led to the same improvement of performance as it has in the control of mechanical and electrical systems, paper attempts to explain why; complexity of chemical processes, lack of suitable measuring equipments, remote objectives i.e. out of 1000 variables only 10 are of interest, modes not always easily separated; proposes matrix method in which important modes are picked out for control.

(S-33)-14.

(C-11) Cadman, Rothfus & Kermode - uses matrix methods and frequency response techniques for design of multicomponent feedforward control system.

32. Hybrid Computer Control

(D-13) Dahlin & Nelson - uses hybrid computer and matrix maximum principle for optimal control.

33. Analog Computer Control

(J-6)-20.; (K-2)-21.; (L-3)-15.; (R-3)-18.; (H-15)-22.

(L-14) Lupfer & Oglesby - elaborate analog controller described, instrumentation and feedback schemes.

(L-6) Luyben & Gerster - studies effectiveness of feedforward control for 10 and 40 tray columns, performance of overhead and bottoms controller determined by analog simulation and by experimental tests on a 10 tray - 2 ft. column; concludes that

relatively simple feedforward controllers appear adequate for distillation; for small input disturbance, a linear model can be used to determine controller transfer functions.

(W-27) Williams & Harnett - uses frequency response analysis, plate equations, first order lags; describes various control schemes.

34. Optimal Control

(L-9) Lapidus - nonlinear optimal control, quadratic performance criteria, Riccati equation and solution, etc.

(B-11) Brosilow & Handley - optimal control of the overhead composition of a distillation column, integral squared error criterion on disturbances; experimental analysis on 5 inch column with 15 trays and 3 bubble caps per tray; control system behaved well in spite of model inaccuracies.

(B-32)-13.; (A-11)-25.; (D-13)-32.; (K-5)-25.; (S-33)-14.; (J-5)-21.

35. Distributed or Modal Control

(D-9)-16.; (J-6)-33.; (S-31)-43.; (F-16)-12.

(G-13) Gavalas - eigenvalue solutions for distributed parameter steady state.

B2.4 MATHEMATICS AND COMPUTATION

36. Ordinary Differential Equation Theory

(H-11) Hartman - $20.00 text, ordinary differential equations in all aspects from a pure mathematics standpoint, theorem-proof presentation.

(B-14) Birkhoff & Rota - very good presentation of transformations and eigenfunction expansions for two-point boundary-value problems and Sturm-Liouville problems.

(I-2) Ince - if one were ever restricted to only one look on ordinary differential equations, this would have to be the one.

(H-12) Hildebrand - very practical applied mathematics text, useful theory of infinite series expansions to solve DE's.

37. Partial Differential Equation Theory

(G-7) Garabedian - theory of 1st and 2nd order PDE's, basics of integral equation theory, very few examples or problems.

(F-11) Forsythe & Wasow - practical numerical methods text, useful for solving PDE's.

(B-21) Berg & McGregor - very clear presentation of basic principles and solution techniques for PDE's.

(O-1)-21.; (F-12)-17.; (F-16)-12.

(G-6) Gurel & Lapidus - extensive discussion of stability of ODE's and PDE's.

(W-7) Webster - large number of practical example-problems solved.

(H-28) Hildebrand - newest Hildebrand text, seems to be as practical and understandable as the previous texts; numerical methods for solving PDE's.

38. Integral Equation Theory

(T-3) Tricomi - best text on integral equation theory in literature, complete, readable, very few examples.

(P-4) Petrovskii - good presentation of separable kernel theory and use of algebraic equations to approximate integral; several classifying examples and problems.

(L-8) Lovitt - very clear presentation of basic theory with large number of easily worked and instructive examples and problems.

(H-13) Hildebrand - very explicit presentation of methods to convert from IE's to DE's with examples.

(D-5) Davis - large number of methods and equations solved which are not found anywhere else in the literature.

(M-6) Mikhlin - very readable text, terminology sometimes different from standard U.S., coveres about same material as (L-8).

(S-11) Smithies - rigorous text, presents theory of IE's in terms of Lebesgue integration and L_2 spaces; Riemann integration and R_2 spaces are subcases of L_2spaces.

(V-4) Volterra - original classic in theory of integral equations.

(G-7)-37.; (W-7)-37.

(W-6) Whittaker & Watson - very clear, but abbreviated, presentation of IE theory; extensive presentation of infinite series expansions.

39. Mathematical Transformations

(T-4) Tranter - basic theory and application of different types of integral transforms.

(Z-1) Zemanian - recent text, extensive theory of transformations and integral transforms.

(S-31)-43.; (M-16)-44.; (R-14)-21.; (C-8)-21.

40. Matrix Mathematics

(A-4) Acrivos & Amundson - transient solution to column discrete equations by matrix methods, e^{At} solution; this paper referenced very often in the literature; paper originally brought the subject of matrices to the attention of chemical engineers, wide variety of chemical engineering problems solved in this

paper by matrix methods including the absorber problems of (A-1) and (L-2).

(A-12) Amundson - good presentation on eigenfunction expansions; matrix theory.

(H-13)-38.; (J-7)-5.

41. Numerical Solution Techniques

(B-30) Berry & DePrima - develops iterative procedure for the determination of the eigenvalues and eigenfunctions associated with the solution of Sturm-Liouville problems in a finite interval; presents and discusses convergency of an iterative scheme different from "sweeping" or Rayleigh-Ritz; presents numerical example.

(R-24) Ralston - very practical and widely referenced text, many of the programs in the Scientific Subroutine Package (I-3) use methods of this text.

(D-8)-16.; (H-28)-37.; (F-11)-27.; (B-32)-13.

(F-2) Fox - somewhat dated but clear presentation, verified with many numerical examples, of methods for finding boundary-value solutions and eigenvalues.

(K-1) Kenneth & McGill - gradient methods, general numerical methods, some theorems on existence and uniqueness of boundary-value solutions.

(L-10) Liu - numerical solution by finite-difference method; shown to be explicit, stable, more accurate than Crank-Nicholson; solves heat equation and several nonlinear examples.

(M-22) McGinnis - solves Taylor Diffusion type equations using Runge-Kutta techniques; describes numerical methods for BV problems.

(S-13)-21.; (C-8)-21.; (A-10)-5.; (P-8)-5.

(H-19) Hamming - very practical and extensive numerical methods text.

(M-4) McCracken & Dorn - application of numerical methods, flow charting, basic Fortran, programming principles, ODE's and PDE's numerical methods, etc.

(R-4) Rose, Johnson & Williams - used both analog and digital computer to solve plate equations for a 7 plate binary column; found that the time required for the column to change from one steady-state to another after an abrupt change in feed composition is a strong function of the magnitude of change, α, reflux ratio, N, feed tray location; numerical methods used described briefly.

(R-29)-3.; (P-12)-3.; (H-25)-21.; (J-7)-5.; (A-17)-3.

(L-11) Lee - invariant imbedding approach; classical methods use quasi-linearization; invariant imbedding considers a family of problems from zero to the duration of the original problem, by imbedding, solve for the missing conditions for 2-point BV problem; solves Taylor Diffusion type equation as an example.

(D-9)-16.; (M-2)-43.; (R-17)-1.; (J-5)-21.

(N-1) Naylor - numerical solution techniques.

(W-26) White - method for numerically calculating eigenvalues and eigenvectors of large dimension matrices; good bibliography.

(D-15)-16.; (S-12)-5.

42. Boundary Value Problems

(B-8) Boyce & DiPrima - basic text on practical solution techniques and theory of boundary and eigenvalue problems.

(B-9) Beltrami & Wohlers - very theoretical presentation; existence and uniqueness theorems for boundary value problems.

(V-1) Villadsen & Stewart - new collocation methods given for solving symmetrical boundary-value problems using orthogonality conditions to select collocation points; accuracy is shown to be comparable to least squares or variational methods, calculations are much simpler; applications given to one-dimensional eigenvalue problems and to parabolic and elliptic PDE's; collocation methods are special techniques for solving integral equations numerically.

(L-11)-41.; (H-11)-36.; (K-1)-41.; (B-14)-36.; (M-22)-41.;
(B-32)-13.; (F-2)-41.; (H-12)-36.; (H-25)-21.

43. Eigen-Values, Vectors, and Functions

(S-31) Singer - state variable transformations and matrix methods to select significant modes and eigenvalues of multivariable systems.

(M-2) Mickley, Sherwood & Reed - numerical solutions of PDE's using finite differences applied to stagewise processes; orthogonal functions and infinite series solutions of PDE's.

(B-30)-41.; (A-12)-40.; (G-13)-35.; (H-11)-36.;
(H-13)-38.; (I-2)-36.; (B-14)-36.; (D-3)-19.;
(S-13)-21.; (V-1)-42.; (W-26)-41.; (B-5)-22.;
(H-12)-36.; (J-7)-5.

44. Special Functions

(A-18) Abramowitz & Stegun - complete and extensive analytical, numerical, and graphical presentations of special functions.

(L-23) Lebedev - practical user's text showing mathematical properties of special functions and examples of usage.

(M-16) Magnus, Oberhettinger & Soni - states and proves many of the mathematical properties of special functions.

(R-28) Rainville - similar to (L-23).

45. Computation and Computer Programming

(O-4) Organick - basic principles of Fortran IV in textbook form with large number of examples.

(I-3) Scientific Subroutine Package - set of over 250 subroutines for performing standard numerical manipulations such as matrix inversion, integration, differentiation, expansion in functions, least squares curve fitting, roots of polynomials, etc.; (I-3) is in Fortran IV but recently (1969) a reduced package in PL/I has been released.

(M-4)-41.; (P-8)-5.; (H-29)-28.; (M-18)-5.; (B-15)-1.

SECTION 2

MODELS OF BINARY DISTILLATION COLUMNS (M)

M1 THE DISCRETE-PLATE EQUATIONS (DPE)

M2 THE CONTINUOUS-SPATIAL EQUATION (CSE)

M3 SOLUTION TECHNIQUES FOR THE CSE

M4 LINEAR APPROXIMATIONS TO THE CSE

"I HAVE HARDLY EVER KNOWN A MATHEMATICIAN WHO WAS CAPABLE OF REASONING." — PLATO

"PLATO WAS A FOOL!" — JACKIE GLEASON

THIS SECTION PRESENTS DISCRETE AND CONTINUOUS MODELS FOR THE COMPOSITION BEHAVIOR OF A BINARY PLATE DISTILLATION COLUMN. THE CONTINUOUS-SPATIAL EQUATION (CSE) IS DEVELOPED FROM THE DISCRETE-PLATE EQUATIONS (DPE) BY CONSIDERING THE PLATE NUMBER TO BE A CONTINUOUS VARIABLE. SOLUTION METHODS FOR THE CSE ARE PRESENTED, INCLUDING TRANSFORMATIONS, GENERAL SOLUTION TECHNIQUES, NONLINEAR APPROXIMATIONS, AND LINEAR APPROXIMATIONS. AS A FINAL RESULT THE LINEAR POLYNOMIAL-COEFFICIENT MODEL (LPCM), WHICH IS THE SUBJECT OF SECTION 3, IS DEVELOPED AS A LINEAR APPROXIMATION TO THE CSE.

CHAPTER M1

THE DISCRETE-PLATE EQUATIONS (DPE)

The development of the discrete dynamic model of a binary plate distillation column is the subject of this chapter. The development begins by defining the symbols to be used in the derivation. Then the individual plate equations will be developed by considering component mass balances on a typical plate. Finally several comments are made referencing the literature pertaining to the discrete-plate equations. The developments of this chapter are a simplified version of those presented in reference (G-3).

The symbols to be used in the derivation of the individual plate equations are presented in Table M1.1. These symbols are to be applied to the characteristics of the idealized, typical plate of the lower or stripping section of the column as shown in Figure M1.1. The derivation of the equation for the rectification or upper section are identical except that the upper flow constants must be used. The author has attempted to keep these symbols consistent with those used in Chapters I1 and I2 and especially in Table I2.1.

The dynamic model is a system of equations developed for each plate by utilizing the basic principle of conservation of mass stated in Equation M1.1. The four possible mass balances which can be applied

$$\text{Accumulation} = \text{Inflow} - \text{Outflow} \qquad \text{M1.1}$$

to the plate of Figure M1.1 are listed below. Three of these mass balances, numbers 2, 3, and 4 are satisfied by the assumptions stated in Table M1.1 for the individual variables. These assumptions restrict

u_n - Concentration of the lighter component in n-th plate liquid (lbm mole lighter component/lbm liquid)

$f(u_n)$ - Concentration of the lighter component in the n-th plate vapor (lbm mole lighter component/lbm vapor)

α - Relative volatility (dimensionless); assumed constant

F - Feed rate (lbm liquid/hour); assumed constant

D - Distillate rate (lbm liquid/hour); assumed constant

W - Bottoms withdrawal rate (lbm liquid/hour); assumed constant

H - Liquid holdup on the plate (lbm liquid); assumed constant

h - Vapor holdup above the plate (lbm vapor); assumed constant

L_u - Liquid rate in the rectification section (upper section) (lbm liquid/hour); assumed constant

L_l - Liquid rate in the stripping section (lower section) (lbm liquid/hour); assumed constant

V - Vapor rate in the column (lbm vapor/hour); assumed constant

B_u - Upper reflux ratio, L_u/V, (lbm liquid/lbm vapor)

B_l - Lower reflux ratio, L_l/V, (lbm liquid/lbm vapor)

k - Feed plate index (integer)

n - Internal plate index (integer), $1 \leq n \leq N$

N - Total number of plates in the column (integer)

E - Murphree plate efficiency (dimensionless), defined by Equation I2.1, E = 1 assumed for all plates

q - Portion of the feed which adds to the lower liquid rate; $L_l = L_u + qF$; further developments use q = 1, saturated liquid feed

Table M1.1 - LIST OF SYMBOLS USED IN DISTILLATION COLUMN DYNAMIC MODELS

1. Liquid phase mass balance of the lighter component.
2. Liquid phase overall mass balance.
3. Vapor phase mass balance of the lighter component.
4. Vapor phase overall mass balance.

the overall validity of the model greatly but are utilized to simplify the developments which follow in later chapters. It is eventually expected that the generality of the Linear Polynomial-Coefficient Model (LPCM) presented in Section 3 can be utilized to generate solutions which are nearly as accurate in representing the essential nature of the column transient behavior as would be a completely general model using four equations per plate.

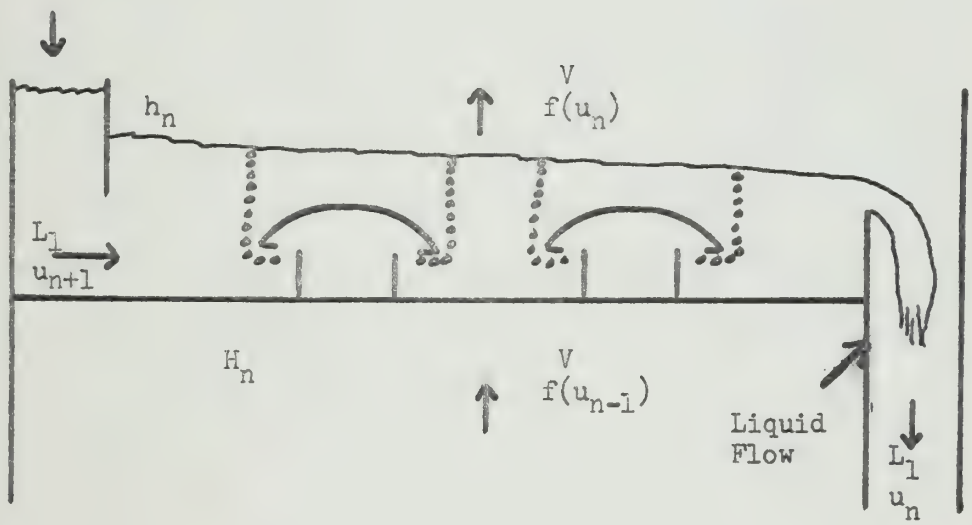


Figure M1.1 - TYPICAL RECTIFICATION PLATE WITH SYMBOLS

The mass balance of the lighter component in the liquid phase gives equation M1.2 for the upper section and M1.3 for the lower section. The steady-state portions of these equations are seen to be equivalent to the discrete-plate steady-state equations in Figure I2.3.

$$H \frac{du_n}{dt} = V \left[f(u_{n-1}) - f(u_n)\right] + L_u\left[u_{n+1} - u_n\right] \quad \text{M1.2}$$

$$H \frac{du_n}{dt} = V \left[f(u_{n-1}) - f(u_n)\right] + L_l\left[u_{n+1} - u_n\right] \quad \text{M1.3}$$

The overall binary distillation column dynamic model utilizing the discrete-plate equations can now be presented as Figure M1.2, where the effects of the condenser and reboiler have not been included. It can be seen that this model consists of N-nonlinear ordinary differential equations with boundary conditions. This particular model is a highly simplified version of the more general models (using all 4 equations with varying holdups and flow rates) usually considered in the literature (See B2.2 - Discrete Plate Equations). The solution techniques to be applied to the continuous-spatial equation developed in later chapters can also be applied to more general models; but for the purposes of presenting the LPCM and its solution techniques, the model of Figure M1.2 is sufficient. When accurate quantitative behavior is desired, the discrete-plate model is almost always the model employed in the control system applications described in the literature (B2.3 - Digital Computer Control).

The reader is referred to the very extensive literature in Chapters B1 and B2 for further information pertaining to discrete-plate models and solutions. This chapter has presented a very brief

development of the discrete-plate model (DPM) for the purpose of utilizing it in the development of the continuous-spatial model (CSE) which is subsequently to be linearized to the linear polynomial-coefficient model (LPCM) for which an analytical solution procedure is developed. The next chapter presents the development of a continuous-spatial model (CSE) from this discrete-plate model.

Model Equations

Rectification Section $\quad k + 1 \leq n \leq N$

$$H \frac{du_n}{dt} = V \left[f(u_{n-1}) - f(u_n)\right] + L_u \left[u_{n+1} - u_n\right]$$

Feed Tray $\quad n = k$

$$H \frac{du_k}{dt} = V \left[f(u_{k-1}) - f(u_k)\right] + L_u u_{k+1} - L_l u_k + F u_f$$

Stripping Section $\quad 1 \leq n \leq k - 1$

$$H \frac{du_n}{dt} = V \left[f(u_{n-1}) - f(u_n)\right] + L_l \left[u_{n+1} - u_n\right]$$

Equilibrium

$$f(u_n) = \frac{\alpha u_n}{1 + (\alpha - 1) u_n}$$

End Conditions

$f(u_n) = u_d \quad$ Top $\quad n = N$

$u_1 = u_w \quad$ Bottom $\quad n = 1$

Feed and Flow Conditions

$L_l = L_u + qF \quad$ or $\quad B_l = B_u + qF/V$

$V = L_u + D$

$W = L_l - V$

Figure M1.2 - THE DISCRETE-PLATE EQUATIONS FOR A BINARY PLATE DISTILLATION COLUMN

CHAPTER M2

THE CONTINUOUS-SPATIAL EQUATION

This chapter presents the steps in the procedure used to transform the discrete-plate equations of Figure M1.2 to the continuous-spatial equation (CSE) which is a continuous dynamic model of the concentration behavior of a binary plate distillation column. In general this conversion represents a significant step away from the quantitative accuracy of the discrete models because of the series expansions and approximations involved. Usually, however, the solutions of the discrete models require comparatively large amounts of time to calculate, often on the order of half (about 15 minutes) of the major concentration time constant (B2.2 - Digital Computer). This makes such models of limited usefulness in control systems which utilize the model to predict transient response in order to correct for transients ahead of time. For these reasons a model is sought which requires less computation time to predict the dynamic response of the distillation column.

The continuous-spatial equation (CSE) may be such a model. The remainder of this thesis will be devoted to developing, investigating, approximating, and solving models of the continuous-spatial type. These models are not expected to behave quantitatively as near to the actual column response as do the discrete models, but it is anticipated that some sacrifice in numerical accuracy will result in a great savings in computation time and therefore better prediction for use in control.

The literature pertaining to continuous models is somewhat limited. The best single presentation on this subject in the literature of Chapter B1 is by Rosenbrock (R-12). It would seem that the most general

form of continuous model solved analytically in the literature is the Taylor Diffusion Model (Chapter L4) which results from approximations which, for the case of distillation, have been shown not to represent accurately the behavior of the column (G-3) (R-7). The most general form of continuous model solved numerically in the literature is the polynomial-class nonlinear model (Chapter M3). This model is solved by numerical methods which treat the continuous variable as a set of discrete points, and therefore the solution takes nearly as much time as solving the discrete equations (B2.2 - Transient or Time Analysis). It can be expected that most of the time savings resulting from solving continuous models will be a direct result of extensive analytical analysis and judicious approximation. This will be the objective of the following chapters in this thesis.

The development of the continuous-spatial equation begins with the representation of the plate number n by a continuous-spatial variable x given in equation M2.1. The variable x is continuous from

$$x = gn \qquad \text{M2.1}$$

Where: n = plate number
g = plate spacing (ft.)

bottom to top of the column. The general discrete-plate equation is represented here from Chapter M1 as equation M2.2. The transformation

$$H \frac{du_n}{dt} = Vf(u_{n-1}) - Vf(u_n) + Lu_{n+1} - Lu_n \qquad \text{M2.2}$$

Where: $u_n = u_n(t)$

from plate number to spatial variable means that u_n is redefined as

in equation M2.3 and M2.4. Using these functions, equation M2.2 now becomes the partial differential equation of M2.5.

$$u_n(t) = u(x,t) \qquad \text{M2.3}$$

$$u_{n+1}(t) = u(x+g,t) \qquad \text{M2.4}$$

$$H\frac{\partial u(x,t)}{\partial t} = Vf\,[u(x-g,t)] - Vf\,[u(x,t)] + Lu(x+g,t) - Lu(x,t) \qquad \text{M2.5}$$

The continuous-spatial equation M2.5 is as exact as the discrete-plate equation M2.2, only it is in a different form. Equation M2.5 is too general for any analytical solution, thus, the terms in x-g and x+g are each expanded in a Taylor Series (G-3), and up to the second order terms are retained as in equations M2.6 and M2.7. If these are now substituted into equation M2.5 the result is given by equation M2.8.

$$Vf\,[u(x-g,t)] = Vf\,[u(x,t)] - gV\frac{\partial}{\partial x} f\,[u(x,t)] + \frac{g^2V}{2}\frac{\partial^2}{\partial x^2} f\,[u(x,t)] \qquad \text{M2.6}$$

$$Lu(x+g,t) = Lu(x,t) + gL\frac{\partial f}{\partial x}\,[u(x,t)] + \frac{g^2L}{2}\frac{\partial^2}{\partial x^2} u(x,t) \qquad \text{M2.7}$$

$$H\frac{\partial u}{\partial t} = \frac{g^2}{2}\frac{\partial^2}{\partial x^2}\,[Lu + Vf(u)] + g\frac{\partial}{\partial x}\,[Lu - Vf(u)] \qquad \text{M2.8}$$

Equation M2.8 can be written in a somewhat neater form with the use of several variable changes. Dividing through M2.8 by V

and considering t in all of the above equations to be $t = t_c$, where t_c is the column time variable, then the transformation to a new time variable t is given by M2.9. Similarly the continuous spatial variable

$$t = \frac{V}{H} t_c \qquad \text{M2.9}$$

of the column is considered to be x_c, and the change of variable on x is given by equation M2.10. If the condenser and the reboiler are

$$x = x_c/g \qquad \text{M2.10}$$

now considered as the 0'th and N + 1'st plates respectively, then the ranges of the variables can be scaled as in M2.11 and M2.12, with the column height represented by C_h (ft.) in M2.13 for equally spaced plates.

$$0 \leq x_c \leq C_h \qquad \text{M2.11}$$

$$0 \leq x \leq 1.0 \qquad \text{M2.12}$$

$$C_h = (N+1)g \qquad \text{M2.13}$$

If all of these operations are applied to equation M2.8, the result is equation M2.14.

$$\frac{\partial u}{\partial t} = \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[Bu + f(u)\right] + \frac{\partial}{\partial x} \left[Bu - f(u)\right] \qquad \text{M2.14}$$

The complete model of the distillation column composition dynamic behavior using continuous spatial equations (CSE) can now be presented as Figure M2.1. This chapter has presented the steps in the procedure used to convert the DPE model of Chapter M1 to the CSE model of Figure M2.1. The CSE model is a highly nonlinear partial differential equation of second order with nonlinear boundary conditions and as such

requires that approximations be made before any analytical results can be expected. Linear approximations to this model are the main subjects of the remainder of this thesis. The next chapter describes possible solution techniques applicable to the CSE and develops the Linear Polynomial-Coefficient Model (LPCM).

Model Equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[Bu + f(u)\right] + \frac{\partial}{\partial x}\left[Bu - f(u)\right]$$

Where: $B_u = L_u/V$ Upper $x_f \leq x \leq 1.0$

$B_l = L_l/V$ Lower $0 \leq x \leq x_f$

x_f = feed tray location

Equilibrium

$$f(u) = \frac{\alpha u}{1+(\alpha-1)u}$$

Boundary Conditions

$$\frac{\partial u}{\partial x} = f(u) - u \qquad x = 1.0 \quad \text{Top}$$

$$B\frac{\partial u}{\partial x} - \frac{\partial f(u)}{\partial x} = \frac{F}{V}(u-u_f) \qquad x = x_f \quad \text{Feed}$$

For: $B_u = L_u/V$ and $B_l = L_l/V$

$$B\frac{\partial u}{\partial x} = f(u) - u \qquad x = 0.0 \quad \text{Bottom}$$

Figure M2.1 - THE CONTINUOUS-SPATIAL EQUATION (CSE) DYNAMIC MODEL

CHAPTER M3

SOLUTION TECHNIQUES FOR THE CONTINUOUS-SPATIAL EQUATION (CSE)

This chapter presents a discussion of possible solution techniques applicable to the CSE, with particular emphasis on a nonlinear approximation to the LSE. The basic equation of the CSE is here repeated for convenience as equation M3.1. The CSE is a second-order, nonlinear, partial-differential boundary-value problem with nonlinear boundary conditions. An outline of possible techniques for solving the CSE is presented in Figure M3.1. In this chapter Parts A, B, C, and E of Figure M3.1 are discussed very briefly, and Part D is examined with the aim of developing the Linear Polynomial-Coefficient Model (LPCM), which is examined in detail in Section 3(1).

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[Bu + f(u)\right] + \frac{\partial}{\partial x}\left[Bu - f(u)\right] \qquad \text{M3.1}$$

As stated previously, any distillation column model would consist of two separate CSE's of the form M3.1: one for the rectification or upper section of the column and one for the stripping or lower section. The two separate CSE's are connected by the boundary condition at the feed tray, which represents the dividing point between the lower and upper sections of the column. Any complete solution for the dynamic composition behavior of a distillation column would therefore involve combining the solutions from two CSE's and their appropriate boundary conditions. The central problem to be considered now is that of solving the CSE.

In order for the reader to get some idea of how complicated the CSE really is, the equation is presented in expanded form as equation M3.2. Considering Part E of Figure M3.1, the general theory of partial differential equations (B2.4 - Partial Differential Equation Theory) provides little help in finding the solution to the CSE. The general theory presents extensive and valuable results pertaining to existence of solutions, characteristic analysis, and methods of solution for linear, semi-linear, and quasi-linear equations, none of which can be applied to the completely nonlinear CSE.

$$\frac{\partial u}{\partial t} = \frac{1}{2}\left[B + \frac{\partial f(u)}{\partial u}\right]\frac{\partial^2 u}{\partial x^2} + \left[\frac{1}{2}\frac{\partial^2 f(u)}{\partial u^2} \cdot \frac{\partial u}{\partial x}\right. \qquad \text{M3.2}$$

$$\left. - \frac{\partial f(u)}{\partial u} + B\right]\frac{\partial u}{\partial x}$$

Where: $u = u(x,t)$, B = constant = L/V

$$f(u) = \frac{\alpha u}{1 + (\alpha-1)u}$$

$$\frac{\partial f(u)}{\partial u} = \frac{\alpha}{[1 + (\alpha-1)u]^2}$$

$$\frac{\partial^2 f(u)}{\partial u^2} = \frac{2\alpha(1-\alpha)}{[1 + (\alpha-1)u]^3}$$

Concerning Part A of Figure M3.1, it would seem to be equally difficult to simulate the entire set of discrete-plate equations as to simulate the CSE by any of the three methods listed. In fact, since the CSE is a partial differential equation, use of digital, hybrid, or analog equipment to simulate it requires that the CSE be broken up into discrete-spatial parts. Some time savings might result in application of an analog computer for the nonlinear spatial portion evaluated at discrete times.

A. Computer Simulation of the CSE

1. Digital Simulation

2. Hybrid Simulation

3. Analog Simulation

B. Application of Transformations to the CSE

1. General Transform Theory

a. Frequency Transforms; Laplace, Fourier, etc.

b. Integral Transforms

2. Change of Variables in the CSE to produce:

a. More Easily Solved Nonlinear Equation

b. Linear Equation

c. More Easily Approximated Equation

C. Application of Some Results in Pure Mathematics to the CSE

1. Contraction Mappings and The Fixed Point Theorem

2. Techniques for Finding the Fixed Point

D. Approximation Techniques for the CSE

1. Nonlinear Polynomial Approximations

2. Linearization and Linear Polynomial-Coefficient Models (LPCM) of the CSE

E. Application of the Theory of Partial Differential Equations to the CSE

Figure M3.1 - POSSIBLE SOLUTION TECHNIQUES FOR THE CSE MODEL

Solution of the CSE by application of some form of transformation to the variables, Part B in Figure M3.1, is one area which might offer rewards with further investigation. Of course, frequency

transforms such as Laplace or Fourier can be eliminated from consideration immediately in the case of the general CSE because they depend upon linearity properties. However, these techniques might be effectively applied to the linearized CSE, and in fact, they are used for analytical and numerical solutions in the literature (B2.2 - Continuous Spatial Equations - Frequency Analysis.)

In the application of a general transformation, an equation of the form M3.3 is sought which will make the CSE a more easily solved nonlinear equation, a linear equation, or a more easily approximated nonlinear equation. In addition, a variable transformation of the form

$$F(s) = \int_0^1 f(u)K(s,u)du \qquad M3.3$$

of equation M3.4 could be applied to the CSE. The resulting complete set of possible transformations on dependent variables is then given by M3.5. Transformations of this type are often used successfully for

$$u = h(v) \qquad M3.4$$

$$F(s) = \int_0^1 f[h(v)]\, K(s,v)dv \qquad M3.5$$

solving problems in fluid mechanics and heat transfer. A search of these areas for transformations applicable to the CSE or some nonlinear approximation to the CSE might prove rewarding.

Part C of Figure M3.1 presents an area of analysis which may possibly apply to a theoretical examination of the CSE. The major consideration here is the use of the Fixed Point Theorem of Brower (S-21) (H-11) to prove such properties as existence, uniqueness, and

continuity of solutions to the CSE. A description of the Fixed Point Theorem depends upon the concept of a contraction mapping. The application of a contraction mapping to the CSE depends upon considering the CSE as a nonlinear differential equation of the form of equation M3.6 at each instant of time.

$$\frac{du}{dx} = f(x,u) \qquad \text{M3.6}$$

The next step in applying the Fixed Point Theorem is the conversion of M3.6 to an integral equation (B2.4 - Integral Equation Theory) presented in equation M3.7. Then the right hand side of M3.7 can be

$$u(x) = u(x_o) + \int_{x_o}^{x} f[z,u(z)]dz \qquad \text{M3.7}$$

considered as a general functional transformation (mapping of functions) A(v) given by equation M3.8. Equation M3.7 can next be written as a functional mapping of the function v onto the function u as in M3.9.

$$A(v) = v_o + \int_{x_o}^{x} f(z,v)dz \qquad \text{M3.8}$$

$$A(v) = u \qquad \text{M3.9}$$

Now, any functional transformation A(u) which satisfies equation M3.10 for any two functions $u_1(x)$ and $u_2(x)$ is defined to be a contraction mapping. The Fixed Point Theorem of Brower (1912) then guarantees

$$|A(u_1) - A(u_2)| \leq M |u_1 - u_2| \qquad \text{M3.10}$$

Where: $0 < M < 1$

for any contraction mapping that there exists a function u, the fixed

point in the mapping, such that M3.11 is satisfied. In other words the function transforms to itself. Equation M3.11 is equivalent to

$$A(u) = u \qquad \text{M3.11}$$

equation M3.7, and thus the Fixed Point Theorem proves existence of a solution to this special case of the CSE if the CSE when written as a transformation can be shown to be a contraction mapping.

The answer to the question of whether the CSE represents a contraction mapping or not could only be determined by further detailed investigations of the CSE. However, since in the original column the variable u represented the concentration of the lighter component in the liquid, it could certainly be expected that u(x,t) would always remain in the range of M3.12. Any distillation column model which has negative or greater-than-unity concentration solutions cannot be valid. In addition, all of the analytical solutions to approximate versions of the CSE in Chapter L4 satisfy equation M3.12.

$$0 \leq u(x,t) \leq 1.0 \qquad \text{M3.12}$$

The Fixed Point Theorem offers valuable information concerning the existence of a solution to a general nonlinear differential equation, but it says nothing about the techniques for finding that solution. It is expected that general solution techniques for an equation involving transformations and contraction mappings would have to be found in the mathematics literature (general topology) and applied to the CSE as a special case. It is highly unlikely that any such techniques could be applied to the CSE without some simplifying

assumptions or approximations being made.

Thus, the analysis of the CSE now proceeds to Part D of Figure M3.1, beginning with nonlinear polynomial approximations to the CSE. The essence of nonlinear approximations lies in the assumption that the equations generated by approximating the coefficients of equation M3.2 using the initial steady-state distribution will be valid for the transient behavior of the column. The validity of this assumption can only be determined by solving specific examples by numerical methods and comparing them to the CSE numerical solutions.

One possible nonlinear approximation technique would be the use of n-th degree polynomials to represent the coefficients of equation M3.2. The steady-state equation would then be a polynomial class (D-5, Ch.8) nonlinear ordinary differential equation of the form of equation M3.13. The resulting nonlinear approximate model of the CSE would be given by equation M3.14, where the p_i and q_i are determined by approximating the coefficient functions of u and the equilibrium relationship by polynomials of sufficient degree for desired accuracy.

$$A(u)\frac{d^2u}{dx^2} + B(u)\frac{du}{dx} + C(u)\left(\frac{du}{dx}\right)^2 + D(u) = 0 \qquad \text{M3.13}$$

Where: $A(u) = \sum_{i=o}^{m} A_i u^i$

$B(u) = \sum_{i=o}^{n} B_i u^i$

$C(u) = \sum_{i=o}^{p} C_i u^i$

$D(u) = \sum_{i=o}^{q} D_i u^i$

A_i, B_i, C_i, D_i are functions of x

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[P_1(u)\right] + \frac{\partial}{\partial x}\left[P_2(u)\right] \qquad \text{M3.14}$$

Where: $P_1(u) = \sum_{i=o}^{n} p_i u^i$

$P_2(u) = \sum_{i=o}^{m} q_i u^i$

The nonlinear approximated version of the CSE presented in M3.14 is an analytically unsolvable equation in general. That M3.14 can be solved using less computation time than that necessary for the CSE is very doubtful. It may be that M3.14 for specific cases might be more easily programmed on an analog computer, but further investigation for specific cases would be required to determine so.

This chapter has presented a brief discussion of a variety of different methods which could be applied to the CSE. The results of the investigation are as expected; in order to proceed with any analytical analysis of the CSE, the equation must be linearized. The development of linearization techniques is presented in the next chapter (M4).

CHAPTER M4

LINEAR APPROXIMATIONS TO THE CONTINUOUS-SPATIAL EQUATION (CSE)

This chapter presents the steps in the linearization procedure to convert the CSE to a linear partial differential equation with spatially varying coefficients. The spatially varying coefficients are then approximated by n-th order polynomials in x, forming the Linear Polynomial-Coefficient Model (LPCM). The most important characteristic of linearized models is that the variable u(x,t) in the linearized model represents the incremental distribution resulting from the linearization about steady-state operation.

The CSE is written in equation M4.1 in terms of $u_c(x,t)$, where $u_c(x,t)$ is the column concentration of the lighter component in the liquid. If M4.1 is linearized about the initial steady-state operation using equation M4.2, then the resulting linearized CSE model for u (x,t) representing the column deviation from the initial steady-state distribution resulting from transient boundary condition variations is given by M4.3. The details of the linearization procedure are presented in Figure M4.1. Equation M4.3 can then be written as a linear partial

$$\frac{\partial u_c}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[Bu_c + f(u_c)\right] + \frac{\partial}{\partial x}\left[Bu_c - f(u_c)\right] \qquad \text{M4.1}$$

$$u_c(x,t) = u_i(x) + u(x,t) \qquad \text{M4.2}$$

differential equation of second-order with spatially varying coefficients by expanding the terms as in equation M4.4.

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[Bu + m(x)u\right] + \frac{\partial}{\partial x}\left[Bu - m(x)u\right] \qquad \text{M4.3}$$

Development of the Linearized CSE

$$A(u) = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[Bu + f(u)\right] + \frac{\partial}{\partial x}\left[Bu - f(u)\right] - \frac{\partial u}{\partial t}$$

$$A(u_c) = A(u_i) + \left.\frac{\partial A}{\partial u}\right|_{u_i}(u)$$

$$u = u_c - u_i$$

$$A(u_i) = A(u_c) = 0$$

$$\left.\frac{\partial A}{\partial u}\right|_{u_i}(u) = 0$$

$$\left.\frac{\partial A}{\partial u}\right|_{u_i} = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[(B + m(x))u\right] + \frac{\partial}{\partial x}\left[(B - m(x))u\right] - \frac{\partial u}{\partial t} = 0$$

Development of the Boundary Conditions

$$A_t(u) = \left(\frac{\partial}{\partial x} - 1\right) f(u) + u = 0 \qquad x = 1.0 \quad \text{Top}$$

Expanding similarly to above:

$$\left(\frac{\partial}{\partial x} - 1\right)(m(x)u) + u = 0$$

$$\left[\frac{dm(x)}{dx} - m(x) + 1\right] u + m(x)\frac{\partial u}{\partial x} = 0 \qquad x = 1.0 \quad \text{Top}$$

$$A_f(u) = B\frac{\partial}{\partial x}\left[u - f(u)\right] - \frac{F}{V}(u - u_f) = 0 \qquad x = x_f \quad \text{Feed}$$

Expanding as above:

$$-\left[B\,\frac{dm(x)}{dx} + \frac{F}{V}\right] u + \left[1 - m(x)\right]\frac{\partial u}{\partial x} = -\frac{F}{V}\,u_f(t)$$

$x = x_f$ Feed

Where: $u_f(t) = u_{fc}(t) - u_{fi}$ Upper and Lower

$$A_b(u) = (B_1\frac{\partial}{\partial x} + 1)\,u - f(u) \qquad x = 0.0 \quad \text{Bottom}$$

Expanding as above:

$$\left[1 - m(x)\right] u + B_1\frac{\partial u}{\partial x} = 0 \qquad x = 0.0 \quad \text{Bottom}$$

Figure M4.1 - DETAILS OF THE CSE LINEARIZATION

$$\frac{\partial u}{\partial t} = \frac{1}{2}\left[B + m(x)\right]\frac{\partial^2 u}{\partial x^2} + \left[B - m(x) + \frac{dm(x)}{dx}\right]\frac{du}{dx}$$

$$+ \left[\frac{1}{2}\frac{d^2m(x)}{dx^2} - \frac{dm(x)}{dx}\right]u \qquad \text{M4.4}$$

It is very important to realize the nature of the function m(x). The function m(x) is defined in equation M4.5 and represents the slope

$$m(x) = \left.\frac{\partial f(u)}{\partial u}\right|_{u = u_i(x)} \qquad \text{M4.5}$$

of the equilibrium curve as a function of x. In equation M4.3 the constant B represents the slope of the operating lines on the McCabe-Thiele diagram of Figure I2.2 in the upper and lower regions. The function m(x) represents the slope of the equilibrium curve in those same regions. Almost all approximation techniques applicable to equation M4.3 use these characteristics and assume that m(x) is given by an equation of the form of M4.6 or M4.8 (R-12) (G-3) (B2.2 - Analytical Analysis). With the assumption of equation M4.6 equation M4.3 becomes equation M4.7 which is the Heat Equation.

$$m(x) = \text{constant} = B \qquad \text{M4.6}$$

$$\frac{\partial u}{\partial t} = B\frac{\partial^2 u}{\partial x^2} \qquad \text{M4.7}$$

It is rather obvious that assumption M4.6 reduces the linearized equation M4.3 to the simplest diffusion equation, thereby neglecting most of the behavior which is unique tc distillation. Distillation is a diffusion process, and it is somewhat reassuring to find that the model M4.3 reduces to a diffusion model. However, it is certain

that a model of the form of M4.7 could not be used to accurately predict column behavior for the purpose of controlling the column. Equation M4.7 is solved analytically and numerically for B = 1.25 in Chapter L4 and represents the "bottom of the ladder" in any hierarchy of approximate models of the CSE.

The next step upward in complexity results from assumption M4.8 resulting in equation M4.3 becoming M4.9. Equation M4.9 is the Taylor Diffusion model equation and is discussed in detail in Chapter L4. This equation is still too approximate to use for any control applications and so, a more sophisticated representation of equation M4.3 is sought.

$$m(x) = \text{constant} \neq B \qquad \text{M4.8}$$

$$\frac{\partial u}{\partial t} = P_1 \frac{\partial^2 u}{\partial x^2} + P_2 \frac{\partial u}{\partial x} \qquad \text{M4.9}$$

Where: $P_1 = (B + m)/2$

$P_2 = (B - m)$

Suppose the spatially varying coefficient functions in equation M4.3 are approximated by n-th degree polynomials in x. Then the resulting complete model would be the Linear Polynomial-Coefficient Model (LPCM) presented in this chapter as Figure M4.2 and in Chapter L1 as Figure L1.1. The boundary function constants A_{ij} in Figure L1.1 are equivalent to the coefficient functions, evaluated at the boundaries, in Figure M4.2.

The central purpose of this thesis is to suggest that the LPCM of Figure M4.2 can be used as a distillation column dynamic model of sufficient accuracy and rapid solution as to be useful in controlling

the column and to present an analytical solution technique for it. This is the subject of Section 3(L).

Model Equations

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left[P_1(x)u\right] + \frac{\partial}{\partial x}\left[P_2(x)u\right]$$

Where: $P_1(x) = \sum_{i=o}^{n} p_i x^i = \left[B + m(x)\right]/2$

$$P_2(x) = \sum_{i=o}^{n} q_i x^i = \left[B - m(x)\right]$$

Upper and Lower Equations, One for Each Section of the Column

Boundary Conditions

$$\left[\frac{dm(x)}{dx} - m(x) + 1\right] u + m(x)\frac{\partial u}{\partial x} = 0 \qquad x = 1.0 \quad \text{Top}$$

$$-\left[B\frac{dm(x)}{dx} + \frac{F}{V}\right] u + \left[1 - m(x)\right]\frac{\partial u}{\partial x} = \frac{-F}{V}u_f(t)$$

$x = x_f$ Feed (Upper and Lower)

$$\left[1 - m(x)\right] u + B_1\frac{\partial u}{\partial x} = 0 \qquad x = 0.0 \quad \text{Bottom}$$

Figure M4.2 - THE COMPLETE LINEAR POLYNOMIAL-COEFFICIENT MODEL (LPCM)

SECTION 3

THE LINEAR POLYNOMIAL - COEFFICIENT MODEL (L)

L1 ANALYTICAL SOLUTION OF THE LPCM BY INTEGRAL EQUATION TECHNIQUES

L2 THE PARTIAL LINEAR POLYNOMIAL BOUNDARY VALUE PROGRAM (PLPBV)

L3 DETERMINATION OF THE LPCM FOR EXAMPLE DISTILLATION COLUMNS

L4 ANALYTICAL SOLUTIONS TO APPROXIMATED COLUMN EQUATIONS

L5 OTHER SOLUTION TECHNIQUES APPLICABLE TO THE LPCM

"DAZZLED BY THEIR ABILITY TO DO ELEMENTARY THINGS AT TREMENDOUS SPEEDS AND TO PUT THESE TOGETHER IN STRUCTURES OF DAUNTING COMPLEXITY, SOME HAVE ALLOWED THE TERM 'GIANT BRAINS' TO GAIN CURRENCY AND, SEDUCED BY THE SIREN SONG OF SO SENSELESS A SOBRIQUET, HAVE SURRENDERED THEIR BIRTHRIGHT OF RATIONAL THOUGHT FOR A POTTAGE OF PUNCHED CARDS." - R. ARIS (A-13)

THE CENTRAL PURPOSE OF THIS THESIS IS THE DEVELOPMENT, PRESENTATION, SUGGESTED SOLUTION TECHNIQUE, AND EVALUATION OF THE LINEAR POLYNOMIAL - COEFFICIENT MODEL (LPCM) OF THE DYNAMIC BEHAVIOR OF A BINARY PLATE DISTILLATION COLUMN. THE FUNCTION OF THIS SECTION IS THE PRESENTATION AND UTILIZATION OF THIS MODEL AND THE DEVELOPMENT OF AN INTEGRAL EQUATION SOLUTION TECHNIQUE FOR IT.

CHAPTER L1

ANALYTICAL SOLUTION OF THE LPCM BY INTEGRAL EQUATION TECHNIQUES

The purpose of this chapter is to present a somewhat involved analytical solution of the Linear Polynomial-Coefficient Model (LPCM) defined by equation L1.1 with boundary conditions L1.2, L1.3, and L1.4. The LPCM is a linear, second-order, parabolic, partial-differential, two-point, boundary-value problem and, as such, cannot be solved analytically or numerically with complete generality (B-8). The best that can be done analytically is to develop a solution technique which allows reasonable assumptions and approximations to greatly simplify the analytical manipulations leading to a simplified solution. The best that can be done numerically is to develop and employ programs specifically related to specialized cases of the LPCM and then to utilize those programs on digital, hybrid, or analog equipment to compute a simplified solution. In either case, the solution may or may not truely represent the behavior of the distillation column from which the model was developed.

Equations of the form of the LPCM are usually solved numerically by a variety of different techniques. Numerical solutions to the LPCM are described in Chapter L5 and a survey of the literature in the Bibliography, Chapter B1, pertinent to solving the LPCM is presented there. No attempts have been made to solve the LPCM in a purely numerical fashion in this thesis, although the suggestion can be made that such attempts might prove to be exceedingly profitable in terms of greatly reduced solution computation time when using the LPCM as part of a column control system.

The solution technique to be described in this chapter is a sequence of analytical manipulations which lead to an expression which is then to be evaluated numerically. The technique begins with expressing the response in terms of steady state and transient portions. The technique of separation of variables is then employed for the transient partial differential equation. The spatial differential equation portion resulting from the separation of variables is then solved by converting it to a Liouville Normal-Form equation and then to a homogeneous Fredholm II-integral equation. The total solution is then expressed in terms of the eigenvalues and eigenfunctions resulting from the solution of the integral equation. The anticipated advantage occuring from these analytical manipulations is that the final numerical evaluation in this technique may take much less computation time than solving the LPCM purely numerically.

L1.1 TRANSIENT AND STEADY-STATE EQUATIONS FROM THE LPCM

The Linear Polynomial-Coefficient Model is defined by equation L1.1 with boundary conditions L1.2, L1.3, and L1.4. This model represents the deviation from steady state of the concentration of the lighter component in the distillation column subject to step changes in the end-point compositions. The complete presentation of the development of this model has been given in Section 2(M).

The first step to be taken in the analytical solution of L1.1 is the realization that, at any given instant of time, there are three separate spatial concentration distributions implied by the model. First of all, there is the initial steady state distribution $u_1(x)$ in the column prior to the step inputs. Since the LPCM

$$\frac{\partial^2}{\partial x^2}[P_1(x)u] + \frac{\partial}{\partial x}[P_2(x)u] = \frac{\partial u}{\partial t} \qquad \text{L1.1}$$

Where: $u = u(x,t)$

$$P_1(x) = \sum_{i=0}^{n} p_i x^i$$

$$P_2(x) = \sum_{i=0}^{n} q_i x^i$$

$$A_{11}u(b,t) + A_{12}u_x(b,t) = A_{13} + A_{14}U_{-1}(t) \qquad \text{L1.2}$$

$$A_{21}u(a,t) + A_{22}u_x(a,t) = A_{23} + A_{24}U_{-1}(t) \qquad \text{L1.3}$$

$$A_{11}A_{22} - A_{12}A_{21} \neq 0 \qquad \text{L1.4}$$

Figure L1.1 - THE LPCM

represents an approximation to an equation which has been linearized about an initial steady state, this portion should be zero if the model is to be valid, but cannot be assumed zero for any general model. Thus, $u_i(x)$ must satisfy equation L1.5 with boundary conditions given by L1.6 and L1.7.

$$\frac{\partial^2}{\partial x^2}[P_1(x)u_i(x)] + \frac{\partial}{\partial x}[P_2(x)u_i(x)] = 0 \qquad \text{L1.5}$$

$$A_{11}u_i(b) + A_{12}\dot{u}_i(b) = A_{13} \qquad \text{L1.6}$$

$$A_{21}u_i(a) + A_{22}\dot{u}_i(a) = A_{23} \qquad \text{L1.7}$$

The second distribution implied by the model is the final steady state $u_s(x)$. This represents the lighter component concentration in the column after the step inputs and after all transients have had

time to die out. The final steady state $u_s(x)$ must also satisfy equation L1.5, but with the boundary conditions given by L1.8 and L1.9.

$$A_{11}u_s(b) + A_{12}\dot{u}_s(b) = A_{13} + A_{14} \qquad \text{L1.8}$$

$$A_{21}u_s(a) + A_{22}\dot{u}_s(a) = A_{23} + A_{24} \qquad \text{L1.9}$$

The third concentration distribution is the transient response $u(x,t)$ - (Note: the same notation is used for the transient response as was used in L1.1 for simplicity) - which must satisfy equation L1.1, but with the boundary conditions L1.10 and L1.11 and the initial condition L1.12. In the interest of having a completely defined problem and also from the practical constraint of proper model behavior, the final condition L1.13 must also be included.

$$A_{11}u(b,t) + A_{12}u_x(b,t) = 0 \qquad \text{L1.10}$$

$$A_{21}u(a,t) + A_{22}u_x(a,t) = 0 \qquad \text{L1.11}$$

$$u(x,0) = u_o(x) = u_i(x) - u_s(x) \qquad \text{L1.12}$$

$$u(x,\infty) = 0 \qquad \text{L1.13}$$

The net result of considering these three spatial distributions is that the LPCM solution now is seen to be the solution of three separate problems: two ordinary differential problems L1.5 with different boundary conditions and one partial differential problem L1.1 with conditions L1.10 - L1.13.

The general usefulness of the LPCM must lie in the capability of using step response solutions to approximate the response to any arbitrary input functions of time. In utilizing the model in this general manner, the initial steady state $u_i(x)$cannot be assumed to be zero and the model must be solved as the three separate problems described previously.

For the purposes of presenting and solving the LPCM in terms of single step inputs, however, the assumption will be made in this thesis that A_{13} and A_{23} are both zero and, thus, that the initial steady state distribution $u_i(x)$ is zero throughout the column, i.e. that the initial deviation from steady state is zero. Solution of the general problem implies solving for $u_i(x)$ in L1.5 and using it, along with $u_s(x)$, in the transient boundary condition L1.12.

The assumption that $u_i(x) = 0$ for the purpose of evaluating the model reduces the solution to one partial differential problem L1.1 in the transient response $u(x,t)$ and one ordinary differential problem L1.5 in the steady state response $u_s(x)$ with boundary conditions given by L1.14 and L1.15. Once the transient and steady state solutions have been determined, the total model solution $u_m(x,t)$ for

$$A_{11}u_s(b) + A_{12}\dot{u}_s(b) = A_{14} \qquad \text{L1.14}$$

$$A_{21}u_s(a) + A_{22}\dot{u}_s(a) = A_{24} \qquad \text{L1.15}$$

step inputs can be expressed as L1.16. Then $u_m(x,t)$ will satisfy the LPCM with $A_{13} = A_{23} = 0$. The development of these solutions begins with the application of the technique of separation of variables to the transient partial differential equation L1.1.

$$u_m(x,t) = u_s(x) + u(x,t) \qquad \text{L1.16}$$

L1.2 SEPARATION OF VARIABLES APPLIED TO THE LPCM

The method of separation of variables rests on the assumption that the solution u(x,t) can be separated into a product of two functions X(x) and T(t) as in eq. L1.17. This assumption is the

$$u(x,t) = X(x) \cdot T(t) \qquad \text{L1.17}$$

single most universally used analytical technique for solving partial differential equations. If this expression for u(x,t) is then substituted into the LPCM, the resulting expression is equation L1.18, where P_3 and P_4 are defined in L1.32 and L1.33.

$$P_1\ddot{X}T + P_3\dot{X}T + P_4XT = X\dot{T} \qquad \text{L1.18}$$

If this expression is divided by XT, then the resulting expression in equation L1.19 represents a function of x equated to a function of t for all values of x and t. Thus, the two expressions must equal a constant - K^2.

The applicability of this technique to a given partial differential equation rests on the capability of separating the

$$\frac{P_1\ddot{X} + P_3\dot{X} + P_4X}{X} = \frac{\dot{T}}{T} = -K^2 \qquad \text{L1.19}$$

resulting equation, as in equation L1.18. This step is, in general, not possible when the given partial differential equation is non-linear as are, for example, the continuous-spatial equation and polynomial-class partial differential equations (Davis, D-5, p.213).

The general condition for separability of a partial differential operator of the form of L1.20 has been shown by Murray-Lasso (M-5) to be the commutation of the operators H_x and H_t expressed in eq. L1.21. In this case H_x, H_t, and $L_{x,t}$ are partial differential operators in x, t, and both x and t, respectively. In the case

$$L_{x,t}\,[u(x,t)] = H_t\,[u(x,t)] + H_x\,[u(x,t)] \qquad \text{L1.20}$$

$$H_x\,[H_t(u)] = H_t\,[H_x(u)] \qquad \text{L1.21}$$

of the continuous-spatial equation H_t and H_x are defined by equations L1.22 and L1.23, where $f(u,u_x,u_{xx})$ is a nonlinear function.

$$H_t\,[u] = \frac{\partial u}{\partial t} \qquad \text{L1.22}$$

$$H_x[u] = f(u,u_x,u_{xx}) \qquad \text{L1.23}$$

That these two operators do not commute is shown in eq. L1.24 and therefore the continuous-spatial equation is not separable. The

$$\frac{\partial}{\partial t}\,[H_x(u)] = \frac{\partial H_x}{\partial t}\,\frac{\partial u}{\partial t} = H_x\,[u_t] \qquad \text{L1.24}$$

LPCM, however, does satisfy eq. L1.21 and is separable, as has been shown in eq. L1.19.

The application of the separability assumption then results in the transformation of the partial differential equation in two variables to a set of two ordinary differential equations, each of which depends upon the separation constant $-K^2$. The two resulting ordinary differential equations are presented as the spatial equation L1.25 and the time equation L1.26.

$$P_1\ddot{X} + P_3\dot{X} + P_4X = -K^2X \qquad \text{L1.25}$$

$$\dot{T} = -K^2T \qquad \text{L1.26}$$

L1.3 SOLUTIONS OF THE TIME EQUATION

The time equation L1.26 is an eigenvalue problem whose eigenfunction solutions are easily found. Since $u(x,t)$ in equation L1.1 represents the transient portion of the desired solution, the separation constant has been chosen as $-K^2$ in order that each eigenfunction of the transient response approach zero for large values of time as in equation L1.13. The eigenfunctions which satisfy equation L1.26 are shown as functions of the eigenvalues $-K_m^2$ in equation L1.27.

$$T_n(t) = \exp(-K_n^2 t) \qquad \text{L1.27}$$

L1.4 SOLUTIONS OF THE SPATIAL EQUATION

The eigenvalue problem presented by the spatial equation L1.25 and its associated boundary conditions is much more difficult to solve than the time equation problem. In fact, statements about the existence, uniqueness, and continuity of solutions for this problem cannot be made in general (B-8). Statements of this nature require restrictions on the equation or the boundary conditions. There are some existence and uniqueness theorems for restricted cases presented in the literature (B-9) (K-1) (H-11), however, the existence, continuity, and completeness of eigenfunction solutions to regular Sturm-Liouville problems will be assumed and utilized in this section (B-14) (I-2).

Several very simple cases of the spatial equation L1.25 can be solved analytically. These simple cases are for P_1, P_3, and P_4 set equal to constants, and examples of these are solved in Chapter L4. In all of these simple cases and, in fact, for the problem L1.25 in general, the final steady state distribution in the transient solution boundary condition L1.12 is expanded in terms of the eigenfunctions of problem L1.25. For reasonably well behaved systems, such as a binary distillation column, it is expected that only the first few, say ten (10) or less, of the eigenvalues are really crucial to the transient behavior of the distillation column. The reason that only the smallest eigenvalues $-K_n^2$ are important to the total transient behavior is that the time-eigenfunctions in equation L1.27 approach zero for very small values of time when the eigenvalues $-K_n^2$ become larger. As mentioned in Chapter L4, the analytical solution evaluations of the simple cases of the LPCM always required less than ten (10) eigenfunctions for three-decimal-place accuracy.

These considerations offer promise of greatly simplified solution expressions for the LPCM if an analytical technique can be developed which offers a solution in terms of the first few eigenvalues and eigenfunctions. As mentioned in Chapter L5, there are numerous analytical and numerical procedures which offer this representation; however, conversion of L1.25 to an integral equation and then solution of the integral equation either by separation of the kernel (Appendix A2) or by approximating the integral equation by a system of linear algebraic equations (Appendix A3) will be investigated in this thesis.

The integral equation technique consists of converting the differential equation to the Liouville Normal-Form equation and then converting the Liouville Normal-Form equation to a Fredholm II-integral equation. The first conversion procedure begins with a test for self-adjointness and a transformation of L1.25 to a regular Sturm-Liouville equation L1.40. The end result of these manipulations is the set of spatial equation eigenvalues K_n in equation L1.49 and the set of eigenfunctions $W_n(z)$ in either equation A2.15 or A3.10 with the transformation relations L1.44, L1.45, L1.37, and L1.39 leading to the eigenfunction solutions $X_n(x)$. The following sections present the development of these transformations and the equation solution procedures.

L1.5 SELF-ADJOINT CONDITIONS AND TRANSFORMATIONS

If the spatial equation L1.25 can be shown to be self-adjoint, then the spatial eigenvalue problem is a regular Sturm-Liouville eigenvalue problem. If the spatial equation is not self-adjoint, then the variables can be transformed into a self-adjoint equation which then represents a regular Sturm-Liouville problem. In an analytical analysis such as employed in this chapter, it is essential that at some step the equations be expressed in a format for which real eigenvalues and complete eigenfunctions are guaranteed. The regular Sturm-Liouville problem is such a format (B-14) (I-2).

The necessary and sufficient condition that the spatial equation L1.28 be self adjoint is expressed by equation L1.29. When this

$$P_1(x)\overset{\bullet\bullet}{X} + P_3(x)\overset{\bullet}{X} + [P_4(x) + K^2]\, X = 0 \qquad \text{L1.28}$$

$$\overset{\bullet}{P}_1(x) = P_3(x) \qquad \text{L1.29}$$

condition is applied to the coefficient polynomials in equations L1.30, L1.31, L1.32, and L1.33, the polynomial coefficient relations L1.34 and L1.35 result. The self-adjoint form of equation L1.28 is then given by equation L1.36.

$$P_1(x) = \sum_{j=1}^{n+1} p_{j-1} x^{j-1} = \sum_{i=0}^{n} p_i x^i \qquad \text{L1.30}$$

$$P_2(x) = \sum_{j=1}^{n+1} q_{j-1} x^{j-1} = \sum_{i=0}^{n} q_i x^i \qquad \text{L1.31}$$

$$P_3(x) = q_o + \sum_{j=1}^{n} (2jp_j + q_j x) x^{j-1} \qquad \text{L1.32}$$

$$P_4(x) = q_1 + \sum_{j=1}^{n-1} (j+1) \left[jp_{j+1} + q_{j+1} x \right] x^{j-1} \qquad \text{L1.33}$$

$$q_{j-1} + jp_j = 0 \qquad j = 1, \cdots, n \qquad \text{L1.34}$$

$$q_n = 0 \qquad \text{L1.35}$$

$$\frac{d}{dx} \left[P_1(x) \dot{X} \right] + P_4(x) X = -K^2 X \qquad \text{L1.36}$$

If the spatial equation L1.28 turns out to be non-self-adjoint, then the transformation relations L1.37, L1.38, and L1.39 (M-2) result in the self-adjoint equation L1.40. This transformed

$$P(x) = \exp \left[\int_a^x \frac{P_3(x)}{P_1(x)} \, dx \right] \qquad \text{L1.37}$$

$$Q(x) = \frac{P_4(x)}{P_1(x)} \cdot P(x) \qquad \text{L1.38}$$

$$R(x) = \frac{P(x)}{P_1(x)} \qquad \text{L1.39}$$

$$\frac{d}{dx} \left[P(x) \dot{X} \right] + Q(x) X = -K^2 R(x) X \qquad \text{L1.40}$$

equation L1.40 is then seen to be of the same form (Sturm-Liouville) as the self-adjoint equation L1.36. The spatial

eigenvalue problem thus reduces to a regular Sturm-Liouville problem with the differential equation expressed by L1.40 and the boundary conditions by L1.41, L1.42, and L1.43.

$$A_{11}X(b) + A_{12}\dot{X}(b) = 0 \qquad \text{L1.41}$$

$$A_{21}X(a) + A_{22}\dot{X}(a) = 0 \qquad \text{L1.42}$$

$$A_{11}A_{22} - A_{12}A_{22} \neq 0 \qquad \text{L1.43}$$

The next step in the solution procedure is to convert the regular Sturm-Liouville equation L1.40 to the Liouville Normal-Form equation L1.46. Equation L1.25 could have been converted directly to an integral equation but this was not done for several reasons. Firstly, the analytical manipulations in the conversion procedure did not lead themselves to the approximation techniques so necessary for finding the final solution. Secondly, and much more importantly, there is no guarantee that a direct transformation would produce an integral equation with a continuous kernel. In fact, in most cases it would not. If either the kernel separation method in Appendix A2 or the linear algebraic method of Appendix A3 were employed for solving an integral equation with a discontinuous kernel, there would be no guarantee that the eigenvalues would be real and distinct. Such a guarantee can be given if the kernel is continuous and symmetric.

L1.6 TRANSFORMATION TO THE LIOUVILLE NORMAL-FORM EQUATION

Transformation on both the dependent and independent variables of equation L1.40 can be used to greatly simplify the regular Sturm-Liouville equation (B-14) (I-2). If new variables W and z are defined

as in equations L1.44 and L1.45, then the equation L1.40 is transformed to that of equations L1.46 and L1.47, where the primes are derivatives

$$X = \frac{W}{4\sqrt{P(x)R(x)}} \qquad \text{L1.44}$$

$$z = \int_a^x \sqrt{\frac{R(x)}{P(x)}}\, dx \qquad \text{L1.45}$$

with respect to x and the equations are expressed as functions of z.

$$\frac{d^2W}{dz^2} + [\lambda - M(z)]W = 0 \qquad \text{L1.46}$$

$$M(z) = \frac{P}{4R}\left[\left(\frac{P^1}{P}\right)^1 + \left(\frac{R^1}{R}\right)^1 + \frac{3}{4}\left(\frac{P^1}{P}\right)^2 + \frac{1}{2}\left(\frac{P^1}{P}\right)\left(\frac{R^1}{R}\right) - \frac{1}{4}\left(\frac{R^1}{R}\right)^2\right] + \frac{Q}{R} \qquad \text{L1.47}$$

Whereas the original equation L1.40 was defined over the interval $a \leq x \leq b$, the transformed equation L1.46 is valid over the interval $0 \leq z \leq c$, where c is defined in equation L1.48 and λ in equation L1.49.

$$c = \int_a^b \sqrt{\frac{R(x)}{P(x)}}\, dx \qquad \text{L1.48}$$

$$\lambda = K^2 \qquad \text{L1.49}$$

The boundary conditions of L1.41 and L1.42 are also transformed to the new boundary conditions on W(z) expressed in equation L1.50 through L1.56, where the dot is d/dz and the prime is d/dx.

$$D_{11}W(c) + D_{12}\dot{W}(c) = 0 \qquad \text{L1.50}$$

$$D_{21}W(0) + D_{22}\dot{W}(0) = 0 \qquad \text{L1.51}$$

$$D_{11} = A_{11} - \frac{A_{12}}{4}\left(\frac{P^1(b)}{P(b)} + \frac{R^1(b)}{R(b)}\right) \qquad \text{L1.52}$$

$$D_{12} = A_{12}\sqrt{\frac{R(b)}{P(b)}} \qquad \text{L1.53}$$

$$D_{21} = A_{21} - \frac{A_{22}}{4}\left(\frac{P^1(a)}{P(a)} + \frac{R^1(a)}{R(a)}\right) \qquad \text{L1.54}$$

$$D_{22} = A_{22}\sqrt{\frac{R(a)}{P(a)}} \qquad \text{L1.55}$$

$$D_{11}D_{22} - D_{12}D_{21} \neq 0 \qquad \text{L1.56}$$

L1.7 SOLUTION OF THE LIOUVILLE NORMAL-FORM PROBLEM

Now that the spatial differential equation L1.28 has been transformed to the Liouville Normal-Form, the next step in the solution of the LPCM consists of finding the eigenvalues λ_i and the eigenfunctions $W_i(z)$ for equation L1.46 with the boundary conditions L1.50 and L1.51. As discussed in subsection L1.4 the technique to be used is that of converting L1.46 to an integral equation and then solving the integral equation.

The conversion procedure is presented in Appendix A1 and two alternative solution procedures are presented in Appendices A2 and A3. The separable kernel procedure presented in Appendix A2 could be employed for specialized cases of the LPCM. The solution procedure in that case would be to approximate the kernel A1.17 by a finite series A2.2 and then to apply the techniques of Appendix A2. This would involve a great deal more analytical analysis for any given LPCM, but it is anticipated that the resulting solutions would be more accurate than those obtained by the methods of Appendix A3. The relative merits of these two solution procedures in terms of solution accuracy and computation time would have to be examined for any given LPCM.

The second integral equation solution procedure in Appendix A3 consists, in essence, of approximating the integral by a finite sum. The procedure is easily programmed on a digital computer and is a very direct method. For these reasons, the procedure in Appendix A3 will be used to evaluate the LPCM in this thesis.

Once the eigenvalues K_n and eigenfunctions $X_n(x)$ of the spatial equation have been found, the next step in finding the total solution to the LPCM is to ensure that the initial condition L1.12 is met. This requires that the initial distribution $u_o(x)$ be expressed in terms of those eigenfunctions $X_n(x)$.

L1.8 THE EIGENFUNCTION EXPANSION

The eigenfunction expansion begins by expressing $u_o(x)$ in equation L1.12 as a sum of constants c_i multiplied by each eigenfunction $X_i(x)$ as in equation L1.57, when n is the number of eigenfunctions. Since

$$u_o(x) = \sum_{i=1}^{n} c_i X_i(x) \qquad \text{L1.57}$$

the integral equation solution technique only gives n eigenfunctions, then equation L1.57 can only be satisfied for n points x_j in the interval $a \leq x \leq b$. Thus, equation L1.57 must be discretized to equation L1.58. Equation L1.58 then represents n-simultaneous equations

$$u_o(x_j) = \sum_{i=1}^{n} c_i X_i(x_j) \qquad \text{L1.58}$$

in n-unknowns which can be expressed as the matrix equation L1.59. The solution to L1.59 is then given by L1.60. Once the matrix C has

$$U_o = XC \qquad \text{L1.59}$$

$$C = X^{-1}U_o \qquad \text{L1.60}$$

been found, the total solution can be expressed in terms of the transient and steady state portions.

L1.9 THE TOTAL SOLUTION TO THE LPCM

The total solution to the LPCM can now be expressed in terms of known functions $u_s(x)$ and $u(x,t)$. The steady state problem L1.5 with boundary conditions L1.14 and L1.15 is a standard linear boundary value problem for which solutions and, in fact, computer subroutines exist. The steady state solution is determined in this thesis by Scientific Subroutine Program - LBVP in reference (I-3) and is described in greater detail in Chapter L2.

The major portion of the LPCM, for which computer programs have not been developed, was the solution to the transient boundary value problem. For this reason, this portion of the LPCM received the greatest portion of solution effort in this thesis. It is expected that the steady state equation could be solved by the same integral equation techniques (leading to a final matrix inversion rather than an eigenvalue problem) as were used for the spatial equation portion of the transient response. The conversion would be more involved because the boundary condition constants A_{14} and A_{24} in equations L1.14 and L1.15 are not zero. The conversion of both the steady state equation and the spatial equation of the transient response, and the incorporation of the solution technique for both of these problems in the same program would undoubtedly result in a great savings of computation time over that spent using the LBVP subroutine and the integral equation techniques separately. This could only be determined from further studies.

The efforts of the previous sections of this chapter have led to the transient solution to the LPCM due to step inputs. The total solution was given in equation L1.16; the transient portion of that solution can now be given as equation L1.61. The total solution to

$$u(x,t) = \sum_{i=1}^{n} c_i X_i(x) \exp(-K_i^2 t) \qquad \text{L1.61}$$

the LPCM is then given by equation L1.62.

$$u_m(x,t) = u_s(x) + \sum_{i=1}^{n} c_i X_i(x) \exp(-K_i^2 t) \qquad \text{L1.62}$$

The next chapter (L2) develops a digital computer program for performing these manipulations and calculating the solution to a special version of the LPCM.

CHAPTER L2

THE PARTIAL LINEAR-POLYNOMIAL BOUNDARY VALUE PROGRAM (PLPBV)

The very general solution technique developed for the LPCM in Chapter L1 is based upon mathematical transformations whose analytical expressions, for general n^{th} order polynomial coefficients, are too complicated to use in a numerical solution evaluation. This chapter presents an application of the integral equation technique of Chapter L1 to the first-degree polynomial model (PLPBV) and a digital computer program for evaluation of the solution.

L2.1 PRESENTATION OF THE MODEL (PLPBV)

The Partial Linear-Polynomial Boundary Value (PLPBV) model is presented in Figure L4.1. This model is a subcase of the LPCM of Figure L1.1 in which $P_2(x)$ is a linear polynomial and $P_1(x)$ is a constant. This model represents one step upward from the simplified LPCM examples of Chapter L4 and, at the same time, the simplest form of the LPCM which still has a spatial varying coefficient.

$$\frac{\partial^2}{\partial x^2}\left[P_1(x)u\right] + \frac{\partial}{\partial x}\left[P_2(x)u\right] = \frac{\partial u}{\partial t} \qquad \text{L2.1}$$

Where: $u = u(x,t)$

$P_1(x) = p_o \; ; \; p_o > 0$

$P_2(x) = q_o + q_1 x$

$$A_{11}u(b,t) + A_{12}u_x(b,t) = A_{14}U_{-1}(t) \qquad \text{L2.2}$$

$$A_{21}u(a,t) + A_{22}u_x(a,t) = A_{24}U_{-1}(t) \qquad \text{L2.3}$$

Figure L2.1 - THE PLPBV MODEL

The development of the solution to this model now parallels that of Chapter L1 for the general LPCM except that the transformation relations can be expressed specifically in terms of the polynomial coefficients.

L2.2 THE TRANSIENT AND STEADY-STATE EQUATION FROM PLPBV

The first step in solving the PLPBV model is the expression of the separate transient and steady-state problems as in subsection L1.1 and equation L1.16. The transient and steady-state problems are presented in detail in Figure L2.2, where $u_m(x,t)$ is the total solution to PLPBV.

$$u_m(x,t) = u_s(x) + u(x,t) \qquad \text{L2.4}$$

Transient Portion:

$$P_1 u_{xx} + P_3 u_x + P_4 u = u_t \qquad \text{L2.5}$$

where: $P_1 = p_o$

$P_3 = q_o + q_1 x$

$P_4 = q_1$

$A_{11}u(b,t) + A_{12}u_x(b,t) = 0$

$A_{21}u(a,t) + A_{22}u_x(a,t) = 0$

$u(x,o) = -u_s(x)$

$u(x,\infty) = 0$

Steady-State Portion:

$$P_1 \ddot{u}_s + P_3 \dot{u}_s + P_4 u_s = 0 \qquad \text{L2.6}$$

where: $P_1 = P_o$

$P_3 = q_o + q_1 x$

$P_4 = q_1$

(Continued on next page)

$$A_{11}u_s(b) + A_{12}\dot{u}_s(b) = A_{14}$$

$$A_{21}u_s(a) + A_{22}\dot{u}_s(a) = A_{24}$$

Figure L2.2 - TRANSIENT AND STEADY-STATE PROBLEMS OF PLPBV

L2.3 SOLUTION OF THE STEADY STATE PROBLEM

The solution of the general LPCM steady state has been discussed in subsection L1.9. The subroutine LBVP, Linear Boundary-Value Problem, and the associated subroutines applicable directly to the general LPCM are presented in Appendix A5 for completeness and for the convenience of the reader. Subroutines LBVP and GELG are taken, less comment cards, directly from the literature (I-3), whereas subroutines AFCT, DFCT, and FCT have been written specifically for the general LPCM. The user must supply his own output subroutine OUTP as per reference (I-3).

Once LBVP is called in the main portion of PLPBV then it calculates the steady-state values $u_s(x_j)$ for use in equations L1.58, for the final transient eigenfunction expansion, and in L1.62, for the total solution evaluation at the discrete points x_j. The user OUTP subroutine must be set up to return $u_s(x_j)$ values to PLPBV at exactly the desired x_j.

Some comments concerning the efficiency of LBVP in the application must be made. It is obvious that since both FCT and DFCT return zero values that a simpler version of LBVP for this special case could be written or possibly found in the existing literature by

further searching. As mentioned in L1.9, the integral equation techniques might also be applied here.

For the initial purposes of evaluating the LPCM and testing the transient portions of PLPBV, the steady state constants were fed in as Column 9, Matrix 3, in Appendix A4. Subroutines LBVP, AFCT, DFCT, and FCT have all been compiled, tested, and shown to operate properly.

L2.4 SOLUTION OF THE TRANSIENT PROBLEM; ANALYTICAL ANALYSIS

The solution to the transient portion of PLPBV defined in Figure L2.2 will be obtained by applying the transformation relationships to L2.5 to convert the spatial equation equivalent to L1.25 to the Fredholm II-Integral Equation A1.21. This analysis will be divided into an analytical analysis in which the specifics of the transformations will be presented and a computational analysis in which subroutine PLPBV will be explained and presented.

The analytical analysis of the transient portion of PLPBV begins with separation of variables. The time equation eigenfunctions resulting from the application of the separation-of-variables technique are the same in PLPBV as they were for the general LPCM in equation L1.27. The resulting spatial equation is given below as equation L2.7.

$$P_1 \ddot{X} + P_3 \dot{X} + [P_4 + K^2] X = 0 \qquad \text{L2.7}$$

where: $P_1 = p_o$

$P_3 = q_o + q_1 x$

$P_4 = q_1$

The next step in the analysis of the spatial differential equation L2.7 is a test to see if the equation is self adjoint or not. If it is self adjoint, then no transformations are necessary because then the equation can be written directly in the form of L1.36. Application of the self-adjoint test conditions L1.34 and L1.35 results in equation L2.8 which shows that equation L2.7 is not self adjoint and that transformations will be required. It is interesting

$$q_1 = 0 \quad , \quad \text{but } q_1 \neq 0 \text{ in PLPBV} \qquad \text{L2.8}$$

to note at this point that $q_1 = 0$ is satisfied for the simplified version of the LPCM solved analytically in Chapter L4 showing that it is already self adjoint.

Since equation L2.7 is non self adjoint, the transformations L1.37, L1.38, and L1.39 can be applied, as in equations L2.9, L2.10, and L2.11, resulting in the self-adjoint equation L1.40. With these functions defined, the second transformation, to the Liouville Normal-Form equation, can be utilized as in equations L2.12 and L2.13 resulting from equations L1.44 and L1.45. Application of transformation

$$P(x) = \exp\left[(x-a)\, q_o/p_o + (x^2-a^2)q_1/2p_o\right] \qquad \text{L2.9}$$

$$Q(x) = P(x)q_1/p_o \qquad \text{L2.10}$$

$$R(x) = P(x)/p_o \qquad \text{L2.11}$$

$$X(x) = W(x)\sqrt[4]{p_o}\ \exp\left[-(x-a)q_o/2p_o - (x^2-a^2)q_1/4p_o\right] \qquad \text{L2.12}$$

$$z = (x-a)/\sqrt{p_o} \qquad \text{L2.13}$$

relations L1.47, L1.48, and L1.49 results, after some manipulations, in equations L2.14, L2.15, and L2.16. Inverting L2.13 and substituting for x in equation L2.14 gives M(z) in L2.17.

$$M(x) = \frac{q_o^2 + 2q_oq_1x + q_1^2x^2}{4p_o} + \frac{3q_1}{2} \qquad \text{L2.14}$$

$$c = (b-a)/p_o \qquad \text{L2.15}$$

$$\lambda = K^2 \qquad \text{L2.16}$$

$$M(z) = \frac{q_o^2 + 2q_oq_1\left(\sqrt{p_o}\,z + a\right) + q_1^2\left(\sqrt{p_o}\,z + a\right)^2}{4p_o} + \frac{3q_1}{2} \qquad \text{L2.17}$$

The next step in the transformation to the Liouville Normal-Form equation is the evaluation of the boundary conditions in L1.50 through L1.55. These relationships are given in equations L2.18 through L2.22.

$$D_{11} = A_{11} - A_{12}(q_o + q_1b)/2p_o \qquad \text{L2.18}$$

$$D_{12} = A_{12}/\sqrt{p_o} \qquad \text{L2.19}$$

$$D_{21} = A_{21} - A_{22}(q_o + q_1a)/2p_o \qquad \text{L2.20}$$

$$D_{22} = A_{22}/\sqrt{p_o} \qquad \text{L2.21}$$

$$D_{11}D_{22} - D_{12}D_{21} = (A_{11}A_{22} - A_{21}A_{12})/\sqrt{p_o} - A_{12}A_{22}q_1\,(b-a)/2p_o^{\frac{3}{2}} \neq 0 \qquad \text{L2.22}$$

The final transformation which must be made is the conversion of the Liouville Normal-Form equation to the Fredholm II-Integral Equation following the steps in Appendix A1. However, all of the functions and constants in equations A1.20 through A1.24 are now known in terms of PLPBV, so the transformation is complete. With these known transformation relationships and with the solution technique of Appendix A3, a digital computer subroutine can be written for computation of the solutions $X_n(x)$, the eigenfunction expansion, and the computation and plotting of the final solution $u_m(x,t)$.

L2.5 SOLUTION OF THE TRANSIENT PROBLEM; COMPUTATIONAL ANALYSIS

Once a complete analytical analysis of any specific subcase of the LPCM has been accomplished, the next step is to write a computer program to evaluate the solutions utilizing analytical transformations and integral equation solution techniques. Such a computer program will require a significant amount of work to write and computation time to check out. However, it is expected that, in the end, the program will require far less computation time than currently available programs which solve the discrete-plate equations. It is expected that a further significant savings in time would result from the design of a special purpose computer to solve a model of sufficient degree to attain desired accuracy for a specific column or type of column.

All computer programs utilizing the methods of this thesis will, by the nature of the method, follow a certain format. This subsection presents a description of the computation steps, in flowchart form,

which this solution method uses. This flowchart is presented in Figure L2.3, and a Fortran IV program listing the details of the block steps in Figure L2.3 for the special case of PLPBV is presented in Appendices A5 and A6.

The PLPBV subroutine presented in Appendix A6 is intended as a description of the steps necessary for solving LPCM problems. Subroutine PLPBV was compiled and executed for several very simplified cases but would require a great deal of work to be useful in general. It is estimated that PLPBV would require between 100 and 200 man-hours of programming time and 1 to 2 hours of computation time to perfect, to consider all special cases, and to debug. The primary benefit from this labor would be the fact that PLPBV only requires about 15 seconds of computation time, and thus, complete column solutions using PLPBV could be generated in less than one minute for 20 spatial points and 9 times.

This chapter has presented a detailed description of the steps necessary to practically apply the general integral equation solution technique developed in Chapter II to a special subcase, PLPBV, of the LPCM. These steps are described analytically by applying the transformation relations to PLPBV and are described numerically by a flowchart of the necessary computation steps and by a very basic Fortran IV digital computer subroutine showing some of the details of the computation steps. The next chapter describes the steps necessary to determine the LPCM for a specific distillation column.

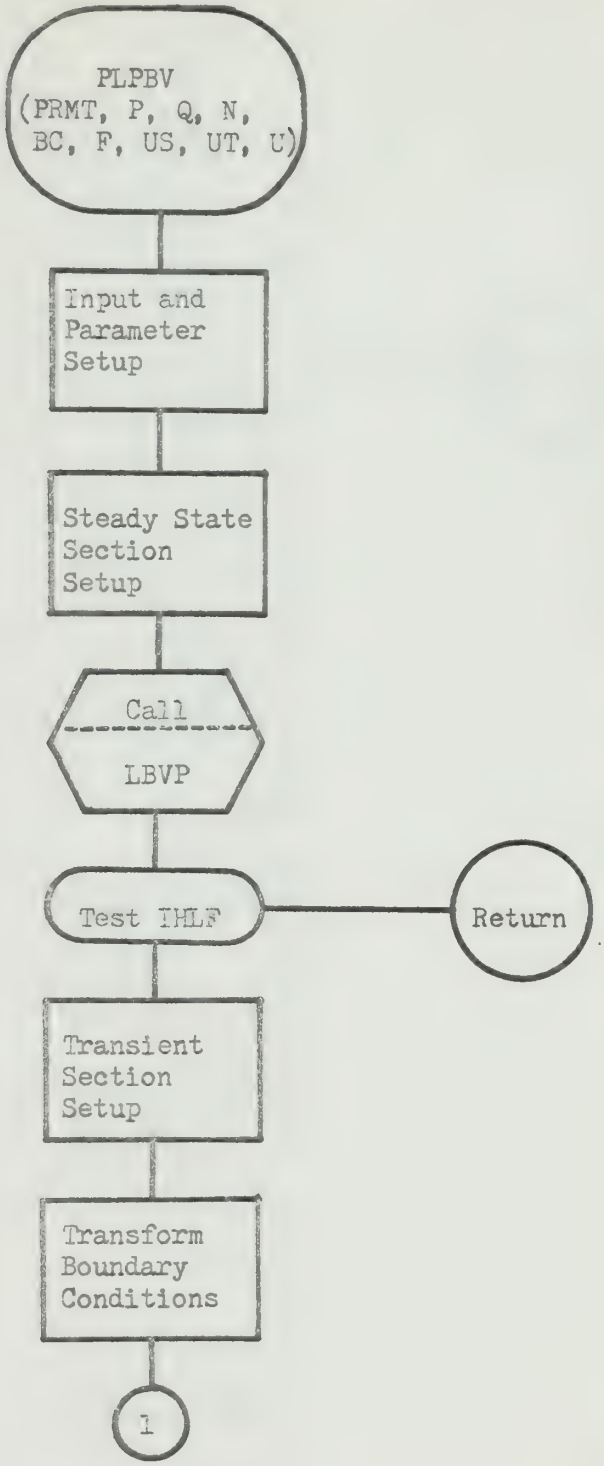


Figure L2.3 (Contd.)

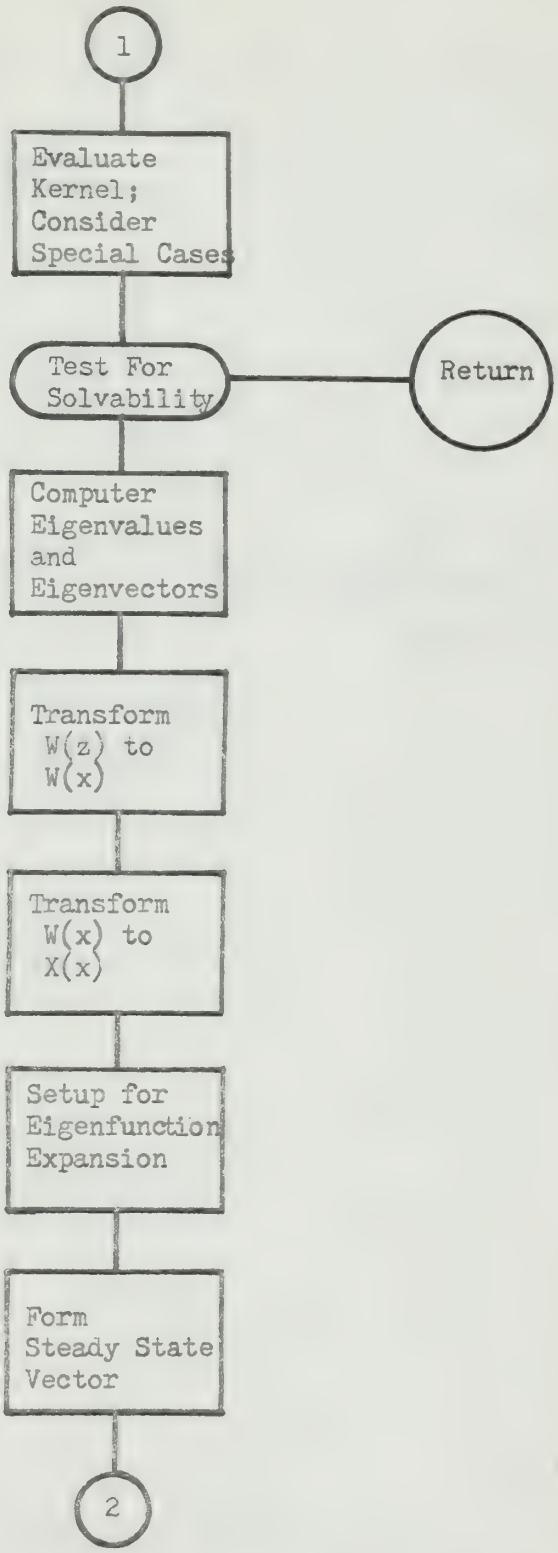


Figure L2.3 (Contd.)

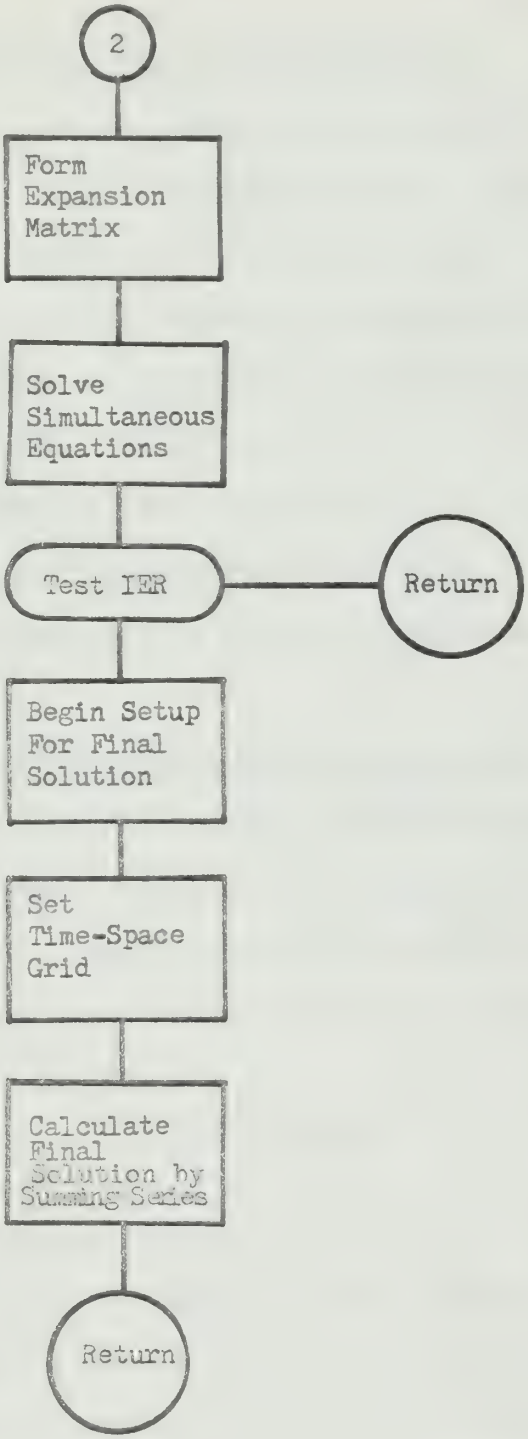


Figure L2.3 - COMPUTATION STEPS IN SUBROUTINE PLPBV

CHAPTER L3

DETERMINATION OF THE LPCM FOR EXAMPLE DISTILLATION COLUMNS

The Linear Polynomial-Coefficient Model (LPCM) has been developed and solved in this thesis as a continuous-spatial model of the transient composition behavior of a binary plate distillation column. The purpose of this chapter is to show the steps required to determine the LPCM for given distillation columns and to discuss the approximations involved in developing the LPCM. Two columns having the same feed and output compositions but different reflux rates and numbers of plates are used as examples to show the development of the LPCM. This chapter represents an equating of Figure M4.2 to Figure L1.1 in terms of the two example columns.

L3.1 GENERAL STATEMENT AND DISCUSSION OF THE MODELING STEPS

The first step in the determination of the LPCM for any distillation column is to determine the slope of the equilibrium curve, $m(x)$, as a continuous function of x. The function $m(x)$ is defined in equation M4.5 and is presented here in detail as equation L3.1. Based upon the

$$m(x) = \left.\frac{\partial f(u)}{\partial u}\right|_{u=u_i(x)} = \frac{\alpha}{[1 + (\alpha-1)u_i(x)]^2} \qquad \text{L3.1}$$

initial steady-state $u_i(x_j)$ represented by the McCabe-Thiele diagram, the function $m(x)$ can be expressed exactly at only a discrete number of points. The major approximation involved in determining the LPCM, aside from the original linearization of the CSE, is the expressing of $m(x)$ as an n-th degree polynomial in x, as in equation L3.2.

$$m(x) = \sum_{i=0}^{n} m_i x^i = m_o + m_1 x + m_2 x^2 + \cdots \qquad \text{L3.2}$$

The continuous-spatial steady-state model has not been explicitly emphasized in this thesis because the direct approximation of the discrete steady-state equilibrium curve slope seems to offer a more direct approach. The continuous steady-state model is equivalent to Figure M2.1 with all time derivatives set equal to zero. If this model were solved for the continuous steady-state $u_i(x)$, then the continuous $m(x)$ could be found from equation L3.1. This is impractical for the LPCM determination because the approximations necessary to develop and solve the continuous steady-state model introduce more error than the direct determination of $m(x)$ from the discrete steady-state model. Thus, continuous steady-state models are not used in this thesis and are very seldom found in the literature.

The accuracy of the LPCM is expected to depend directly upon the accuracy of $m(x)$. Theoretically $m(x)$ can be determined to any desired accuracy using a polynomial in equation L3.2 of sufficiently high degree and using either point-by-point or least-squares techniques. The integral equation solution technique of Chapter L1 is valid for any degree polynomial, but as the degree gets higher than one the transformations become overwhelmingly complicated and the programming time necessary to implement the transformations and consider all of the special bases becomes an order of magnitude larger. Surprisingly enough, the computation time, once the proper programs are written, is not expected to increase significantly over that for PLPBV in Chapter L2 because the basic steps of Figure L2.3 remain nearly the

same and all of the special cases are parallel paths for computation. It is expected that models of degree one or two will prove to be adequate to specify the column behavior sufficiently for the purpose of control.

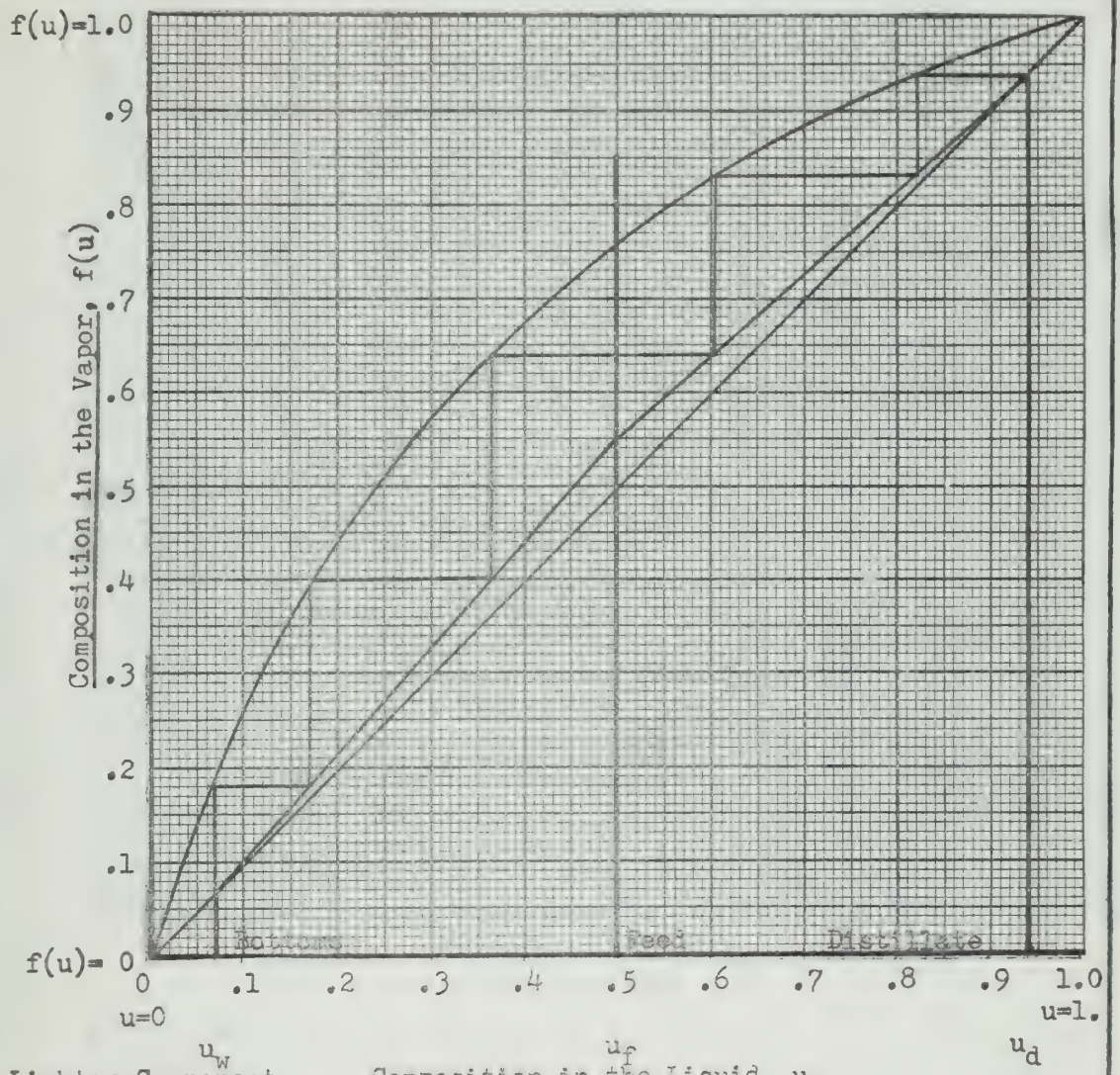
Once the continuous function m(x) has been determined, the model derivation is essentially complete. All that remains is to calculate the polynomial coefficients p_i and q_i and the boundary condition constants A_{ij}. The complete expressions for evaluation of these constants in terms of a second degree m(x) are given in Figure L3.3.

L3.2 APPLICATION OF THE MODELING STEPS TO TWO EXAMPLE COLUMNS

The McCabe-Thiele diagram for a five-plate binary distillation column is presented in Figure L3.1 and the corresponding diagram for an eleven-plate column is presented in Figure I2.2 in Section 1(I). These two diagrams have been designed to have the same input and output compositions to simplify the calculations and to provide for easy comparison. The discrete values of m(x) have been calculated using equation L3.1 and are presented numerically in Table L3.1 and Table L3.2 and presented graphically in Figure L3.2.

x	.0.0	0.2	0.4	0.6	0.8	1.0
n	1	2	3	4	5	6
u_i	0.07	0.17	0.36	0.60	0.82	0.94
m(x)	2.31	1.67	1.01	0.62	0.43	0.36

Table L3.1 - THE DISCRETE m(x) FOR A FIVE PLATE COLUMN



Operating Conditions

Plates = 5
$L_u/V = 0.89$
$L_l/V = 1.06$
$u_f = .50$
$u_w = .07$
$u_d = .94$
$q = 1.0$

Equilibrium Curve

$$f(u) = \frac{\alpha u}{1+(\alpha-1)u}$$

$$\alpha = 3.0$$

Figure L3.1
MCCABE-THIELE DIAGRAM FOR
A FIVE PLATE COLUMN

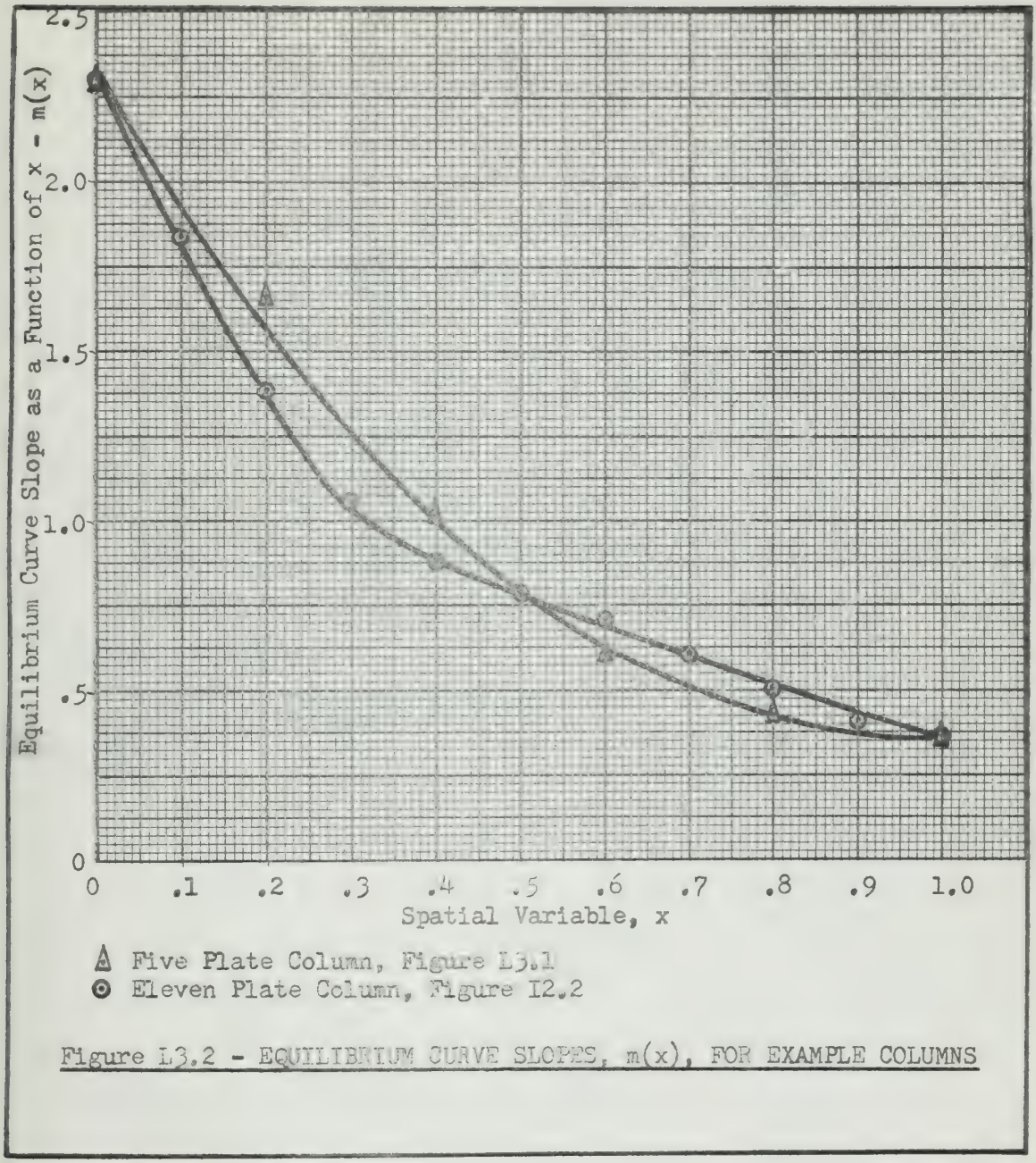


Figure L3.2 - EQUILIBRIUM CURVE SLOPES, m(x), FOR EXAMPLE COLUMNS

Model Equation

$$\frac{\partial^2}{\partial x^2}\left[P_1(x)u\right] + \frac{\partial}{\partial x}\left[P_2(x)u\right] = \frac{\partial u}{\partial t}$$

Where:

$$P_1(x) = p_o + p_1 x + p_2 x^2 = \left[(B + m_o) + m_1 x + m_2 x^2\right]/2$$

Thus: $p_o = (B + m_o)/2$
$p_1 = m_1/2$
$p_2 = m_2/2$

$$P_2(x) = q_o + q_1 x + q_2 x^2 = \left[(B - m_o) - m_1 x - m_2 x^2\right]$$

Thus: $q_o = (B - m_o)$
$q_1 = -m_1$
$q_2 = -m_2$

Both $P_1(x)$ and $P_2(x)$ must be expressed for both the upper and lower sections of the column using B_u and B_l.

Boundary Conditions

Upper
b=1.0
a=x_f

$$A_{11} = \left[\frac{dm(x)}{dx} - m(x) + 1\right]\Bigg|_{x = 1.0}$$

$A_{11} = m_2 - m_o + 1$
$A_{12} = m_o + m_1 + m_2$
$A_{13} = 0$
$A_{14} = 0$

$A_{21} = -\left[B_u\ (m_1 + 2m_2 x_f) + F/V\right]$
$A_{22} = 1 - m_o - m_1 x_f - m_2 x_f^2$
$A_{23} = 0$
$A_{24} = -F/V$

Lower
b=x_f
a=0.0

$A_{11} = -\left[B_l(m_1 + 2m_2 x_f) + F/V\right]$
$A_{12} = 1 - m_o - m_1 x_f - m_2 x_f^2$
$A_{13} = 0$
$A_{14} = -F/V$

$A_{21} = 1 - m_o$
$A_{22} = B_l$
$A_{23} = 0$
$A_{24} = 0$

Feed Condition $F/V = (B_l - B_u)/q$

Figure L3.3 - THE COMPLETE LPCM WITH SECOND DEGREE POLYNOMIALS

x	0.0	0.1	0.2	0.3	0.4	0.5
n	1	2	3	4	5	6
u_i	0.07	0.14	0.24	0.34	0.42	0.48
m(x)	2.31	1.83	1.38	1.06	0.89	0.78

x	0.6	0.7	0.8	0.9	1.0	
n	7	8	9	10	11	
u_i	0.53	0.60	0.71	0.83	0.94	
m(x)	0.71	0.62	0.51	0.42	0.36	

Table L3.2 - THE DISCRETE m(x) FOR AN ELEVEN PLATE COLUMN

The next step in the modeling procedure to develop the LPCM for these two columns is to determine the coefficients of a polynomial, m(x), of sufficient degree to meet accuracy requirements based upon the discrete points given for m(x). In the case of the 5-plate column a polynomial of degree 5 could be found which would exactly match each of the 6 points given, and for the 11-plate column a similar polynomial of degree 10 could be found. However, for both of these columns a 2nd-degree polynomial is expected to be accurate enough. Two second degree polynomials have been found as examples using the points, x = (0.0, 0.2, 1.0), for the 11-plate column and the points, x = (0.0, 0.6, 1.0), for the 5-plate column. The resulting m(x) polynomials are given by equation L3.3 for the 5-plate column and

L3.4 for the 11-plate column.

$$m(x) = 2.31 - 4.17x + 2.22x^2 \qquad \text{5-plate} \qquad \text{L3.3}$$

$$m(x) = 2.31 - 5.32x + 3.37x^2 \qquad \text{11-plate} \qquad \text{L3.4}$$

Once the function m(x) has been determined to the desired accuracy, the complete LPCM for the column can be calculated from the equations of Figure L3.3. The 2nd-degree m(x) polynomials in equations L3.3 and L3.4 result in the complete LPCM for the 5-plate column in Figure L3.4 and the complete LPCM for the 11-plate column in Figure L3.5. It should be emphasized that the approximations and calculations used to obtain equations L3.3 and L3.4 were chosen to greatly simplify the calculations. Normally, the polynomial coefficients for m(x) should be determined specifically for the region of application of the model equation instead of using an overall m(x) as was done in equations L3.3 and L3.4. The column may also be modeled using more sections than the upper and lower sections used in this thesis.

L3.3 GENERAL COMMENTS AND SUMMARY

The real utility of the LPCM results from the fact that as the number of plates in the column increases, the model complexity remains nearly constant for realistic approximations of m(x). The computation time and complexity of discrete models, however, increases rapidly as the number of plates increases because the dimensions of all of the matrices in the model increase with the number of plates. The LPCM is valid for components with non-constant relative volatilities as well as for constant relative volatilities, but only the comstant relative volatility equilibrium curve has been used in this thesis. Also, the

5-PLATE COLUMN

Model Equation

$$\frac{\partial^2}{\partial x^2}[P_1(x)u] + \frac{\partial}{\partial x}[P_2(x)u] = \frac{\partial u}{\partial t}$$

Where: $P_1(x) = p_o + p_1 x + p_2 x^2$
$P_2(x) = q_o + q_1 x + q_2 x^2$

Upper Section		Lower Section	
$p_o = 1.60$	$q_o = -1.42$	$p_o = 1.69$	$q_o = -1.25$
$p_1 = -2.09$	$q_1 = 4.17$	$p_1 = -2.09$	$q_1 = 4.17$
$p_2 = 1.11$	$q_2 = -2.22$	$p_2 = 1.11$	$q_2 = -2.22$

Boundary Conditions

$$A_{11}u(b,t) + A_{12}u_x(b,t) = A_{13} + A_{14}\,U_{-1}(t)$$
$$A_{21}u(a,t) + A_{22}u_x(a,t) = A_{23} + A_{24}\,U_{-1}(t)$$

Upper Section b=1.0, a=0.5

$A_{11} = 0.91$	$A_{12} = 0.36$	$A_{13} = 0.0$	$A_{14} = 0.00$
$A_{21} = 1.57$	$A_{22} = 0.22$	$A_{23} = 0.0$	$A_{24} = -0.17$

Lower Section b=0.5, a=0.0

$A_{11} = 1.90$	$A_{12} = 0.22$	$A_{13} = 0.0$	$A_{14} = -0.17$
$A_{21} = -1.31$	$A_{22} = 1.06$	$A_{23} = 0.0$	$A_{24} = 0.00$

Feed Condition

$F/V = 0.17$

Figure L3.4 - THE COMPLETE LPCM FOR THE 5-PLATE COLUMN OF FIGURE L3.1

LPCM can be used for multiple feed and sidestreams and can be applied in any manner desired to smaller sections of the column. Each subsection of the column can then be modeled using the LPCM.

11-PLATE COLUMN

Model Equation

$$\frac{\partial^2}{\partial x^2}\left[P_1(x)u\right] + \frac{\partial}{\partial x}\left[P_2(x)u\right] = \frac{\partial u}{\partial t}$$

Where: $P_1(x) = p_o + p_1 x + p_2 x^2$
$P_2(x) = q_o + q_1 x + q_2 x^2$

Upper Section $0.5 \leq x \leq 1.0$		Lower Section $0.0 \leq x \leq 0.5$	
$p_o = 1.40$	$q_o = -1.82$	$p_o = 1.92$	$q_o = -0.79$
$p_1 = -2.66$	$q_1 = 5.32$	$p_1 = -2.66$	$q_1 = 5.32$
$p_2 = 1.69$	$q_2 = -3.37$	$p_2 = 1.69$	$q_2 = -3.37$

Boundary Conditions

$$A_{11}u(b,t) + A_{12}u_x(b,t) = A_{13} + A_{14}\,U_{-1}(t)$$

$$A_{21}u(a,t) + A_{22}u_x(a,t) = A_{23} + A_{24}\,U_{-1}(t)$$

Upper Section b=1.0, a=0.5

$A_{11} = 2.06$	$A_{12} = 0.36$	$A_{13} = 0.0$	$A_{14} = 0.00$
$A_{21} = -0.07$	$A_{22} = 0.51$	$A_{23} = 0.0$	$A_{24} = -1.03$

Lower Section b=0.5, a=0.0

$A_{11} = 1.93$	$A_{12} = 0.51$	$A_{13} = 0.0$	$A_{14} = -1.03$
$A_{21} = -1.31$	$A_{22} = 1.52$	$A_{23} = 0.0$	$A_{24} = 0.00$

Feed Condition

$F/V = 1.03$

Figure L3.5 - THE COMPLETE LPCM FOR THE 11-PLATE COLUMN OF FIGURE I2.2

The two models in Figures L3.4 and L3.5 are not solved in this thesis. Their solution will require the development of a computer program based upon the integral equation solution technique of Chapter L1 and using the computation steps of Chapter L2. This will require an

extensive amount of analytical analysis, computer programming, and testing. The result of this labor is expected to be a general, very fast, solution program for the transient behavior of a large class of distillation columns which describes the column behavior accurately enough for control applications. Extensive research would be required to justify this, however.

This chapter presents the steps necessary to derive the LPCM for general distillation columns. The details of these steps are then applied to a 5-plate and an 11-plate column and the resulting LPCM's presented. The next chapter solves analytically and computes numerically the solutions to some simplified LPCM's in which $m(x) = m_o$, a constant.

CHAPTER L4

ANALYTICAL SOLUTIONS TO APPROXIMATED COLUMN EQUATIONS

The purpose of this chapter is to analytically solve and numerically calculate the total solutions to four simple subcases of the Linear Polynomial-Coefficient Model (LPCM) defined in Figure L1.1. The reason for doing this is to provide some examples of simpler solutions upon which to base an understanding of solutions to more sophisticated versions of the LPCM. The procedure to be followed will be to define a simplified version of the LPCM, state the problems to be solved, present the analytical solutions to the problems, present a computer program used to sum the series, and, finally, to present graphically the simplified model solutions.

L4.1 A SIMPLIFIED LPCM

A greatly simplified LPCM is presented in Figure L4.1 by equations L4.1 through L4.5. This model represents one step below the more complicated model presented in Chapter L2. This simplified LPCM appears in many places in the literature, only it is known by the different names and uses listed in Table L4.1, for a representative sample of the literature. This model is usually solved by analytical methods in the literature and used as an example of the application of the method of separation of variables.

L4.2 APPROXIMATE EQUATIONS TO BE SOLVED

There are four specific problems involving the simplified LPCM which will be solved analytically in this chapter. These problems are presented in Figure L4.2 and Table L4.2. Two of the problems involve the solution for the top step response of the heat equation

for the two cases of zero bottoms composition and zero bottoms outflow. The other two problems solved are the Taylor Diffusion Model (TDM) equation for positive and negative values of the center constant q_o.

A visualization of what is happening in terms of distillation column concentration or, by analogy, temperature in a rod is presented in Figure L4.1. If the response desired is the total response to a step change in feed composition, then the equations solved in this chapter apply directly to the bottom half of the column in the range $0 \leq x \leq 1$, where $x = 1$ is the location of the feed tray. The heat analogy would be to visualize a rod with length in the range $0 \leq x \leq 1$ with a step change in temperature at the top.

$$\frac{\partial^2}{\partial x^2}[p_o u] + \frac{\partial}{\partial x}[q_o u] = \frac{\partial u}{\partial t} \qquad \text{L4.1}$$

$$P_1(x) = p_o \qquad \text{L4.2}$$

$$P_2(x) = q_o \qquad \text{L4.3}$$

$$A_{11}u(b,t) + A_{12}u_x(b,t) = A_{14}U_{-1}(t) \qquad \text{L4.4}$$

$$A_{21}u(a,t) + A_{22}u_x(a,t) = 0 \qquad \text{L4.5}$$

Figure L4.1 - A SIMPLIFIED LPCM

AUTHOR(S)	REFERENCE	EQUATION NAME OR USE
Crank	C-8	Diffusion Equation
Gould	G-3	Taylor Diffusion Model (TDM)
Jackson and Pigford	J-1	Transient-Diffusion Equation
Lee	L-11	Convective Transport Equation
Pollock, Brown and Dempsey	P-5	
Stone and Brian	S-13	
Bennett and Meyers	B-1	Heat Equation
Boyce and DiPrima	B-8	
Berg and McGregor	B-21	
Jury	J-2	
Powers	P-7	
Sagan	S-10	
Tsang	T-5	
Woodle	W-14	

Table L4.1 - LITERATURE NOMENCLATURE AND USAGE OF THE SIMPLIFIED LPCM

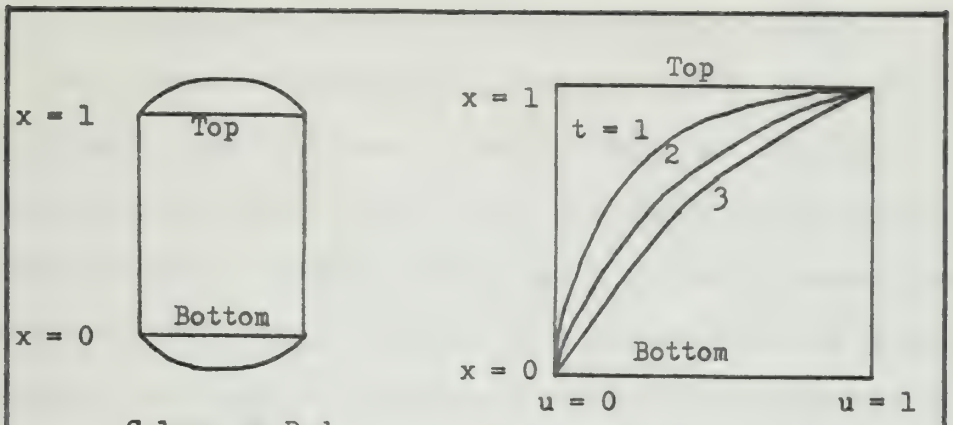


Figure L4.2 - VISUAL AND GRAPHICAL SOLUTION FORMAT

Name	Equation	Equation Name	p_o	q_o	Boundary Conditions A_{11}	A_{12}	A_{21}	A_{22}	A_{14}
UA1	$\alpha^2 u_{xx} = u_t$	Heat	α^2	0	1	0	1	0	1
UA2	$\alpha^2 u_{xx} = u_t$	Heat	α^2	0	1	0	0	1	1
UB1	$\alpha^2 u_{xx} - u_x = u_t$	TDM	α^2	-1	1	0	1	0	1
UC1	$\alpha^2 u_{xx} + u_x = u_t$	TDM	α^2	+1	1	0	1	0	1

Table L4.2 - LPCM PROBLEMS TO BE SOLVED ANALYTICALLY

L4.3 ANALYTICAL SOLUTIONS TO THE SIMPLIFIED LPCM EXAMPLES

This subsection develops the infinite series representations of the analytical solutions to problems UA1, UA2, UB1, and UC1 which have been summarized in Table L4.2. The manipulations leading to these solutions represent no more than a series of mathematical exercises. The details of these solutions are included in this thesis for the sake of completeness and for the convenience of a reader who may want to relate the solution techniques used for the general LPCM solution in Chapter L1 to the much more familiar techniques used in this chapter.

L4.3.1 SOLUTION OF UA1

The total solution to UA1 is given by equation L4.1; the development is presented in the steps below.

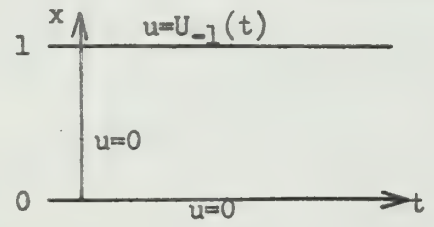
Statement of Problem: Step L4.1

$$\alpha^2 u_{xx} - u_t = 0$$

$$u(1,t) = U_{-1}(t)$$

$$u(o,t) = 0$$

$$u(x,o) = 0$$



Transient plus Steady State: Step L4.2

$$u(x,t) = u_s(x) + u_T(x,t)$$

$$\alpha^2 u_{sxx} = 0 \qquad \alpha^2 u_{Txx} = u_{Tt}$$

$$u_s(0) = 0 \qquad u_T(o,t) = 0 \qquad u_T(x,o) = -u_s(x)$$

$$u_s(1) = 1 \qquad u_T(1,t) = 0 \qquad u_T(x,\infty) = 0$$

Steady State Solution: Step L4.3

$$u_s(x) = x$$

Transient Solution: Step L4.4

$$u_T(x,t) = X(x) \cdot T(t)$$

$$T_n(K) = \exp(-K^2 t)$$

$$X_n(x) = A_1 \cos \frac{K}{\alpha} x + A_2 \sin \frac{K}{\alpha} x$$

$u_T(o,t) = 0$ gives $A_1 = 0$

$u_T(1,t) = 0$ defines eigenvalues $\sin \frac{K}{\alpha} = 0$

gives $K_n = n\pi\alpha$

Eigenfunctions are:

$$a_n \sin(n\pi x) \exp(-K_n^2 t)$$

Expanding to meet the initial condition:

$$u_T(x,0) = -u_s(x) = -x = \sum_{n=o}^{\infty} a_n \sin(n\pi x)$$

Using the orthogonality property of eigenfunctions:

$$\int_o^1 (-x) \sin(m\pi x)dx = \sum_{n=o}^{\infty} a_n \int_o^1 \sin(m\pi x) \sin(n\pi x)dx$$

$$\frac{(-1)^m}{m\pi} = \frac{a_m}{2}$$

Eigenfunction constants:

$$a_n = \frac{2(-1)^n}{n\pi}$$

Transient Solution:

$$u_T(x,t) = 2 \sum_{n=1}^{\infty} (-1)^n \frac{\sin(n\pi x)}{n\pi} \exp\left[-(n\pi\alpha)^2 t\right]$$

Total Solution to UA1:

$$\boxed{u(x,t) = x + 2 \sum_{n=1}^{\infty} (-1)^n \frac{\sin(n\pi x)}{n\pi} \exp\left[-(n\pi\alpha)^2 t\right]} \quad \text{L4.1}$$

L4.3.2 SOLUTION OF UA2

The total solution to UA2 is given by equation L4.2, the development is presented below.

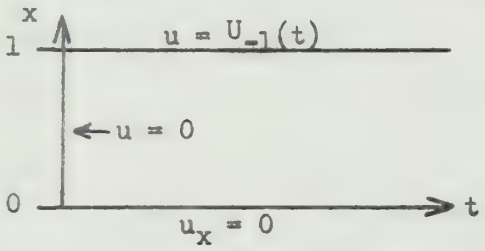
Statement of Problem: Step L4.1

$$\alpha^2 u_{xx} - u_t = 0$$

$$u(1,t) = U_{-1}(t)$$

$$u_x(o,t) = 0$$

$$u(x,o) = 0$$



Transient plus Steady State: Step L4.2

$$u(x,t) = u_s(x) + u_T(x,t)$$

$$\alpha^2 u_{sxx} = 0 \qquad \alpha^2 u_{Txx} = u_{Tt}$$

$$u_s(1) = 1 \qquad u_T(1,t) = 0 \qquad u_T(x,o) = -u_s(x)$$

$$u_{sx}(0) = 0 \qquad u_{Tx}(o,t) = 0 \qquad u_T(x,\infty) = 0$$

Steady State Solution Step L4.3

$$u_s(x) = 1$$

Transient Solution: Step L4.4

$$u_T(x,t) = X(x) \cdot T(t)$$

$$T_n(t) = \exp(-K^2 t)$$

$$X_n(x) = A_1 \cos \frac{K}{\alpha} x + A_2 \sin \frac{K}{\alpha} x$$

$u_{Tx}(o,t) = 0$ gives $A_2 = 0$

$u_T(1,t) = 0$ defines eigenvalues $\cos \frac{K}{\alpha} = 0$

gives $K_n = \frac{n\pi\alpha}{2}$

Eigenfunctions are:

$$a_n \cos\left(\frac{n\pi x}{2}\right) \exp(-K_n^2 t)$$

Expanding to meet the initial condition:

$$u_T(x,0) = -u_s(x) = -1 = \sum_{n=o}^{\infty} a_n \cos\left(\frac{n\pi x}{2}\right)$$

Using the orthogonality property of these eigenfunctions:

$$\int_o^1 (-1) \cos\left(\frac{m\pi x}{2}\right) dx = \sum_{n=o}^{\infty} a_n \int_o^1 \cos\left(\frac{m\pi x}{2}\right) \cdot$$

$$\cos\left(\frac{n\pi x}{2}\right) dx \Rightarrow \frac{\sin(m\pi/2)}{m\pi/2} = -\frac{a_m}{2}$$

Eigenfunction constants:

$$a_n = \frac{-2 \sin(m\pi/2)}{m\pi/2}$$

Transient Solution:

$$u_T(x,t) = -2 \sum_{n=1}^{\infty} \frac{\sin(n\pi/2)}{n\pi/2} \cos(n\pi x/2) \exp\left[-(n\pi\alpha/2)^2 t\right]$$

Total Solution to UA2:

$$u(x,t) = 1 - 2 \sum_{n=1}^{\infty} \frac{\sin(n\pi/2)}{n\pi/2} \cos(n\pi x/2) \exp\left[-(n\pi\alpha/2)^2 t\right] \qquad \text{L4.2}$$

L4.3.3 SOLUTIONS OF UB1 and UC1

The total solutions to problems UB1 and UC1 are given in equations L4.3 and L4.4, respectively. The development of the UB1 solution is presented below; the UC1 solution development is identical to UB1 except for the obvious sign change.

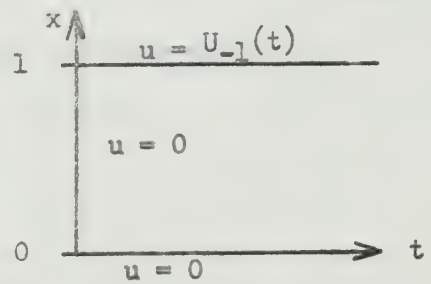
Statement of Problem UB1: Step L4.1

$$\alpha^2 u_{xx} - u_x - u_t = 0$$

$$u(1,t) = U_{-1}(t)$$

$$u(o,t) = 0$$

$$u(x,o) = 0$$



Transient plus Steady State: Step L4.2

$$u(x,t) = u_s(x) + u_T(x,t)$$

$$\alpha^2 u_{sxx} - u_x = 0 \qquad \alpha^2 u_{Txx} - u_{Tx} = u_{Tt}$$

$$u_s(o) = 0 \qquad u_T(o,t) = 0 \qquad u_T(x,o) = -u_s(x)$$

$$u_s(1) = 0 \qquad u_T(1,t) = 0 \qquad u_T(x,\infty) = 0$$

Steady State Solution: Step L4.3

$$u_s(x) = A + B \exp(x/\alpha^2)$$

$u_s(o) = 0$ gives $A + B = 0$

$u_s(1) = 1$ gives $A + B \exp(1/\alpha^2) = 1$

Solving the two A, B equations gives

$$u_s(x) = \frac{1 - \exp(x/\alpha^2)}{1 - \exp(1/\alpha^2)}$$

Transient Solution: Step L4.4

$$u_T(x,t) = X(x) \cdot T(t)$$

$$T_n(t) = \exp(-K^2 t)$$

$$X_n(x) = (A_1 \cos Dx + A_2 \sin Dx) \exp(x/2\alpha^2)$$

$u_T(o,t) = 0$ gives $A_1 = 0$

$u_T(1,t) = 0$ defines eigenvalues $\sin D = 0$ gives $D_n = n\pi$

where: $D_n^2 = \dfrac{4\alpha^2 K_n^2 - 1}{2\alpha^2} = (n\pi)^2$

solving for the eigenvalues

$$K_n^2 = \frac{1}{4\alpha^2} + (n\pi\alpha)^2$$

Eigenfunctions are:

$$a_n \sin(n\pi x) \exp(x/2\alpha^2) \exp(-K_n^2 t)$$

Expanding to meet the initial condition:

$$u_T(x,o) = -u_s(x) = -[1 - \exp(x/\alpha^2)]/C$$

$$= \sum_{n=1}^{\infty} a_n \sin(n\pi x) \exp(x/2\alpha^2)$$

where: $C = 1 - \exp(1/\alpha^2)$

Using the orthogonality with weighting function property of the eigenfunctions:

$$\int_0^1 \left[\exp\left(x/\alpha^2\right) - 1\right] \exp\left(-x/2\alpha^2\right) \frac{\sin(m\pi x)}{C}\, dx$$

$$= \sum_{n=1}^{\infty} a_n \int_0^1 \sin(m\pi x) \sin(n\pi x)\, dx \Rightarrow$$

$$\frac{(-1)^m (m\pi) \exp\left(-1/2\alpha^2\right)}{\left[(m\pi)^2 + (1/2\alpha^2)^2\right]} = \frac{a_m}{2}$$

Eigenfunction constants:

$$a_n = \frac{2(-1)^n (n\pi) \exp\left(-1/2\alpha^2\right)}{\left[(n\pi)^2 + (1/2\alpha^2)^2\right]}$$

Transient Solution:

$$u_T(x,t) = 2 \sum_{n=1}^{\infty} \frac{(-1)^n (n\pi) \exp\left[(x-1)/2\alpha^2\right]}{\left[(n\pi)^2 + (1/2\alpha^2)^2\right]} \sin(n\pi x) \cdot$$

$$\exp\left[-(1/4\alpha^2 + \alpha^2 n^2\pi^2)\, t\right]$$

Total Solution to UB1:

$$u(x,t) = \frac{\left[1 - \exp\left(x/\alpha^2\right)\right]}{\left[1 - \exp\left(1/\alpha^2\right)\right]} + 2 \exp\left[-t/4\alpha^2 + (x-1)/2\alpha^2\right] \cdot$$

$$\sum_{n=1}^{\infty} \frac{(-1)^n (n\pi) \exp\left[-(\alpha n\pi)^2 t\right]}{\left[(n\pi)^2 + (1/2\alpha)^2\right]} \sin(n\pi x)$$

L4.3

Total Solution to UC1:

$$u(x,t) = \frac{\left[1 - \exp\left(-x/\alpha^2\right)\right]}{\left[1 - \exp\left(-1/\alpha^2\right)\right]} + 2 \exp\left[-t/4\alpha^2 + (1-x)/2\alpha^2\right] \cdot$$

$$\sum_{n=1}^{\infty} \frac{(-1)^n (n\pi) \exp\left[-(\alpha n\pi)^2 t\right]}{\left[(n\pi)^2 + (1/2\alpha)^2\right]} \sin(n\pi x)$$

L4.4

L4.4 NUMERICAL CALCULATION AND GRAPHICAL PLOTS OF THE SOLUTIONS

Each of the solutions to the four problems of Table L4.2 contains an infinite series in eigenvalues and eigenfunctions. This section describes briefly a digital computer program which was written and utilized to numerically calculate the values of $u(x,t)$ for $\alpha = 1.18$ at ten spatial points and nine time points. These values were determined for the purpose of making graphical plots of the solutions.

The computer printouts and description of the program are given in Appendix A4. The computer output plots have been used to make the following graphical presentations of the four solutions which are presented in Figures L4.3 through L4.6. It is helpful to visualize these solution curves in terms of Figure L4.2. Each solution curve from left to right represents a spatial distribution at a given time. The curves can be seen to approach their steady state values as, for example, the linear distribution in UA1 or the curved exponential distribution in UC1.

The digital computer program in Appendix A4 computes all four of the solutions to three decimal place accuracy. It was found that at all spatial points and time points the number of eigenvalues and eigenfunctions, i.e. terms in the series, necessary to achieve three decimal place accuracy was in all cases less than ten (10).

L4.5 SIMILARITIES BETWEEN CHAPTER L1 SOLUTIONS AND CHAPTER L4 SOLUTIONS

It is interesting at this point to investigate the similarity between the standard analytical solution methods of this chapter and the general solution technique presented for the LPCM in Chapter L1. This relationship can best be seen by relating each Step in this chapter to the corresponding equations in Chapter L1.

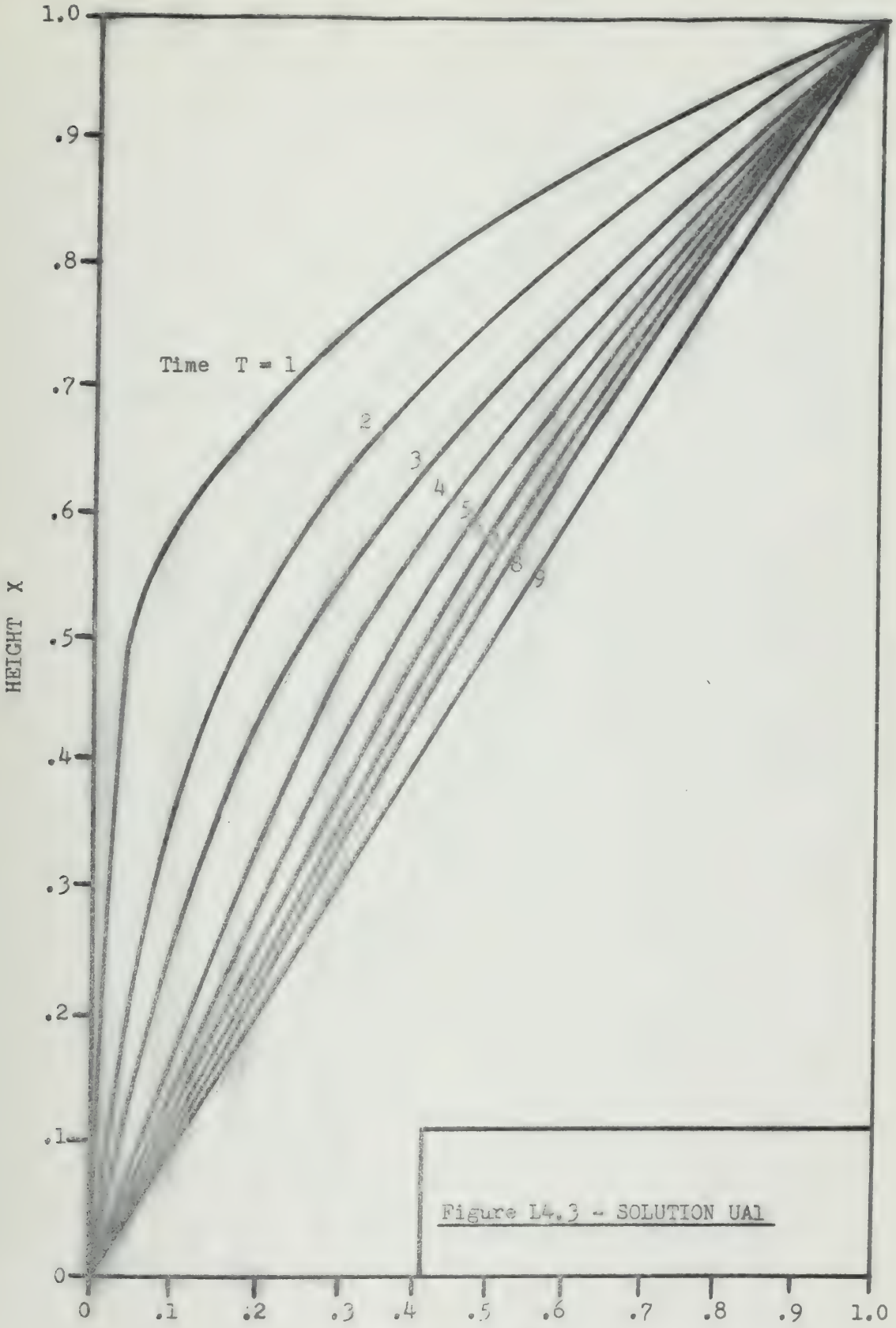


Figure L4.3 - SOLUTION UA1

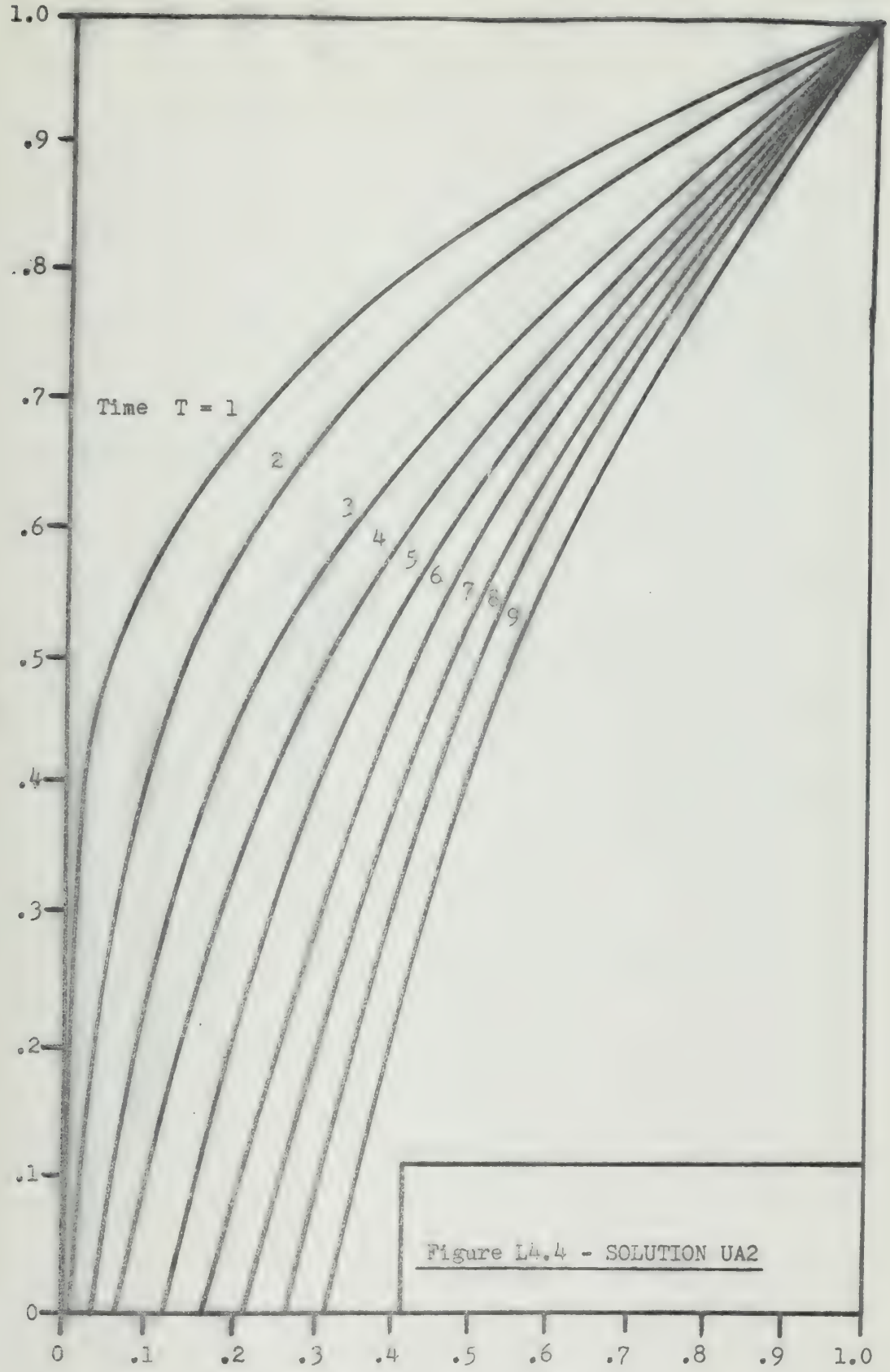


Figure L4.4 - SOLUTION UA2

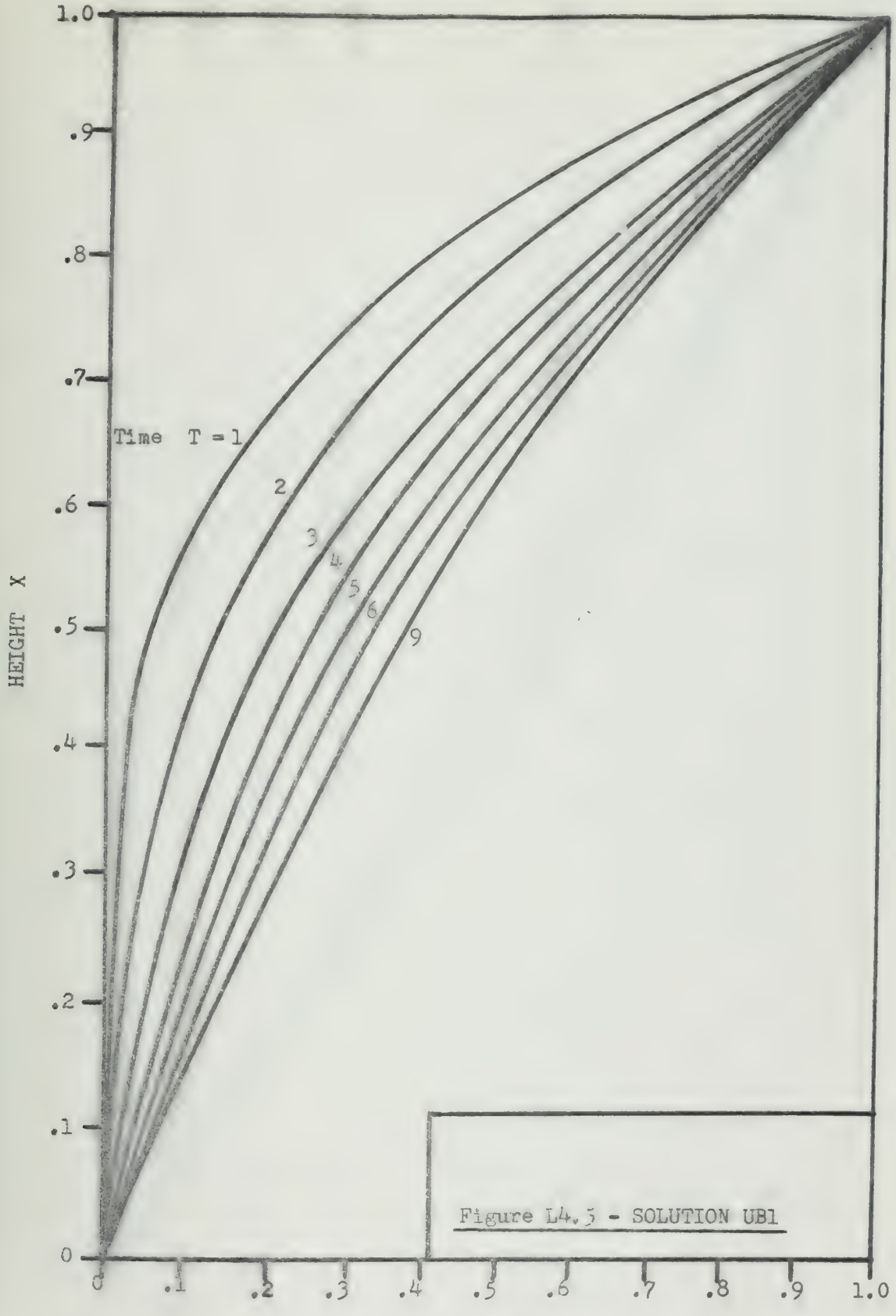


Figure L4.5 - SOLUTION UB1

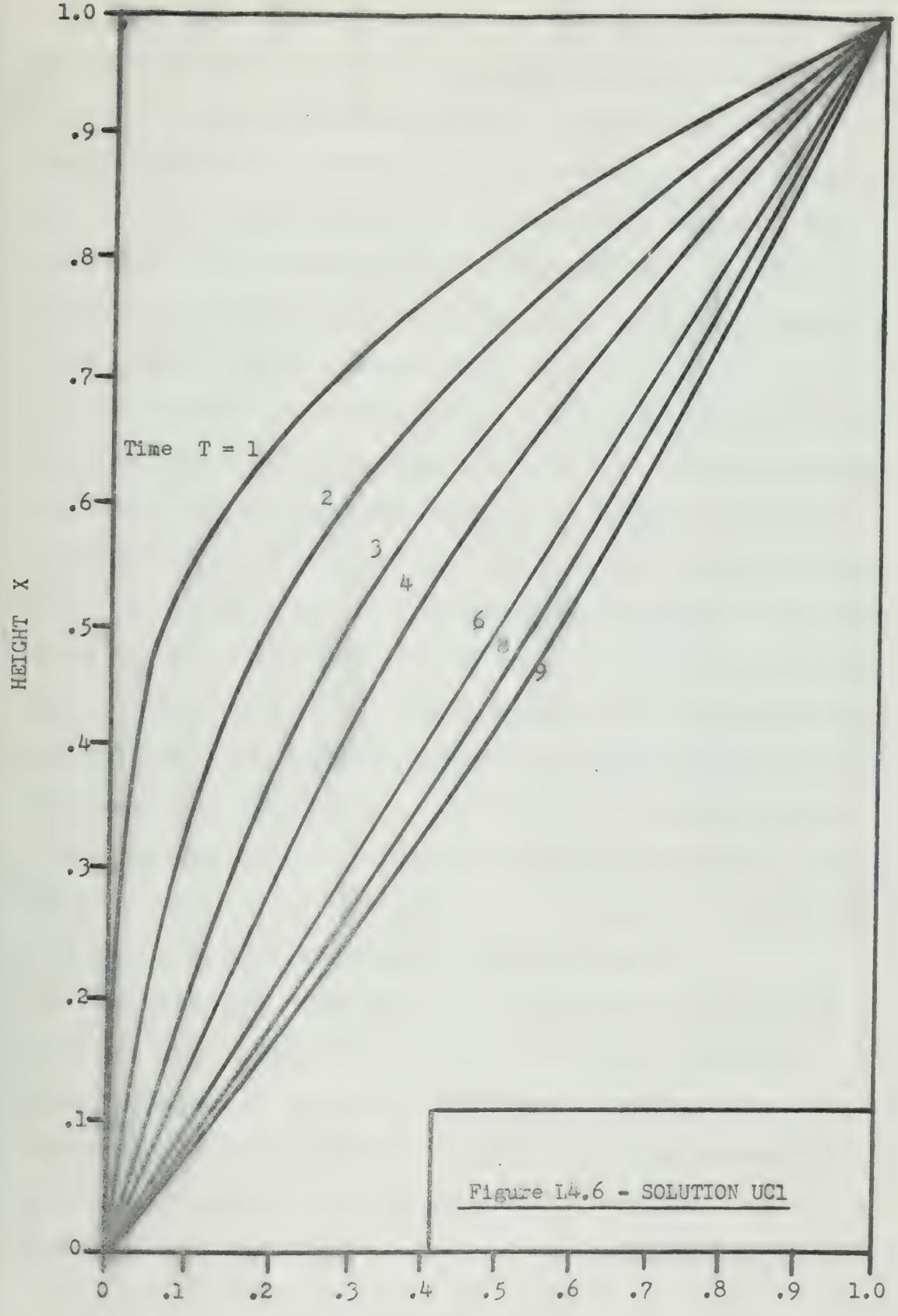


Figure L4.6 - SOLUTION UC1

The problem statement Step L4.1 or, more generally, Figure L4.1 corresponds to Figure L1.1, the statement of the LPCM. The transient and steady state conditions are similar to equation L1.15 and the boundary conditions L1.8 through L1.13. In both cases, the steady state solution, Step L4.3 or L1.5, L1.8, and L1.9, represents the solution to a two point boundary value problem. This is easily found in the simplified equations but requires a computer program (such as LBVP) for the general case.

The transient solution Step L4.4, is, of course, the major step in solving the simplified examples as it is, also, in solving the LPCM in general. In the simplified examples, the eigenfunctions $X_n(x)$ are expressible as closed-form functions with very obvious properties which can be used to satisfy the boundary conditions and to immediately solve for the eigenvalues K_n. In the general LPCM, however, once the equation L1.25 has spatially varying coefficients, the eigenfunctions, in almost all cases, cannot be expressed in closed form but must be represented by infinite series. The infinite series representations of the eigenfunctions can be found by a number of techniques, such as the power series Method of Frobenius (H-12, Ch. 4), but these methods have several major disadvantages in this application.

The first major disadvantage to infinite-series eigenfunction representations is that their properties in terms of satisfying boundary conditions are usually not obvious. Secondly, these methods lend themselves best to specific example solutions and become very difficult to talk about in terms of a general analytical solution technique because of the "special cases" involved. Finally, the

eigenfunction expansion to meet the initial condition is analytically difficult, in general, when these infinite-series eigenfunctions are involved. For these reasons, two other analytical techniques for finding the eigenvalues and eigenfunctions have been investigated.

These two techniques are the Prufer Substitution (B-14, Ch. 11) and Fredholm II - Integral Equation theory (Appendix A1). The Prufer Substitution technique is a transformation applied to the second-order differential equation L1.25 which results in two first order ordinary differential equations whose solutions define the eigenvalues and eigenfunctions. The resulting first order equations are very useful in showing the properties, such as existence, ordinality, separation, orthogonality, etc., of the eigenvalues and eigenfunctions, but the differential equations are analytically untractable in terms of specific solutions and did not seem to lend themselves to consistent approximations. For these reasons the Prufer Substitution has been discarded as a possible analytical solution technique and the integral equation technique has been developed in this thesis.

The final part of the transient solution Step L4.4 is the eigenfunction expansion to meet the initial condition L1.12. The key to success in this expansion for the simplified cases is the orthogonality of the eigenfunctions with respect to a weighting function over the same interval as the boundary conditions are applicable. This orthogonality condition is expressed by equation L4.5. Of course, the sine and cosine functions of the simplified LPCM examples satisfy L4.5. The real utility of the eigenfunction orthogonality condition in the simplified examples lies in the fact that the constants A_n can be each explicitly expressed in terms of n.

$$\int_a^b w(x)\, X_m(x) X_n(x)\,dx = \delta_{mn} C_n \qquad \text{L4.5}$$

where: C_n = constants $\neq 0$

$\delta_{mn} = 0$ for $m \neq n$

$\delta_{mn} = 1$ for $m = n$

One may well wonder why the orthogonality condition was not utilized in solving for the constants C in equation L1.57, when this is one of the most important properties of these functions. The reason is that the functions $X_n(x)$ are the result of transformations L1.44 and L1.45 applied to the solutions $W_i(z)$ obtained from Appendix A2 or Appendix A3 and, as such, are not easily expressed in general form, let alone integrated. For specific cases of the LPCM, if the functions $X_i(x)$ are expressible in a form easily evaluated by integration, then the set of equations L1.59, only with the orthogonality constants instead of the functions evaluated at points x_j, will be individually solvable because the matrix X will be diagonal. In that case, a better solution technique would be to use the orthogonality condition rather than the discrete-point approximate solution technique employed in equation L1.58.

The fact that the functions $X_n(x)$ satisfy the orthogonality condition, in the general case, is a result of the characteristics of the original eigenvalue problem L1.25. If the transformation relations used in subsections L1.5 and L1.6 satisfy continuity conditions and result in the regular Sturm Liouville problem L1.40, then the kernel (A1.17) of the integral equation is guaranteed to be continuous. In addition, it has been shown by Lovitt (L-8, pp. 181-182) that for the special case of $R(x) = 1$ in equation L1.40, the kernel

A1.17 is symmetric and satisfies equation L4.6. The kernel symmetry

$$K(z,s) = K(s,z) \qquad \text{L4.6}$$

guarantees the existence and reality of the eigenvalues and the orthogonality of the eigenfunctions. Of course, in the simplified LPCM examples of this chapter the function R(x) is always one (1).

In summary, this chapter presents analytical and graphical solutions to four simplified cases of the LPCM. The techniques for finding these solutions is then related to the general, integral-equation solution technique for the LPCM presented in Chapter L1. The next Chapter L5 presents a brief discussion of several alternative solution techniques which might be applied to the LPCM.

CHAPTER L5

OTHER SOLUTION TECHNIQUES APPLICABLE TO THE LPCM

This thesis presents the LPCM as a dynamic model of the composition behavior of a binary plate distillation column and suggests an integral equation solution technique for it. The speed and precision of the integral equation solution technique has not been demonstrated completely in this thesis, however. Therefore, this chapter describes briefly the basic principles behind several other numerical methods for the solution of parabolic partial differential equations which might be applied to the LPCM for the purpose of comparing numerical solution accuracy and speed with the integral equation method.

Numerical methods for the solution of ordinary and partial differential equations are extremely useful in the study of distillation columns since both the discrete-plate and the continuous-spatial equations are impossible to solve analytically except in the simplest cases. Even when analytic methods are applicable, it is often the case that the solution is expressed in the form of an infinite series rather than in closed form. When this is the case, it may sometimes be less time consuming to apply a numerical method directly than to evaluate a series to some desired degree of accuracy at each point of interest. This was not true in the simplified cases of Chapter L4 because each of the series converged so rapidly, i.e. less than ten terms.

There are a large number of numerical methods which can be applied to any particular distillation column model, such as the LPCM. The choice of a particular one may depend on the form of the LPCM for any

particular column. This chapter presents the basic principles behind the explicit numerical methods used for solving parabolic partial differential equations, applies these methods to the LPCM, and presents the resulting recursion relations.

L5.1 NUMERICAL SOLUTION TECHNIQUES FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

Parabolic partial differential equations are usually solved by the use of step-by-step finite difference methods (B2.4 - Numerical Solution Techniques). This method consists essentially of defining a regular (usually rectangular) mesh and replacing the differential equation by a difference equation defined on the nodes of the mesh. Most of the variations in types of methods result from different derivations of the difference equation from the differential equation.

In the distillation column models described in Section 2 (M), the solution sought is a function $u(x,t)$ where both u and x are in the 0 to 1 interval and t is greater than zero. A possible mesh for use in equations of this type is presented in Figure L5.1. In this mesh the solution domain is divided into intervals of width h in x and l in t. The two increments h and l need not be the same and in some cases may be changed over different portions of the domains. The ratio of these two increments is constrained by stability requirements for any particular equation and method of solution.

Once the mesh is set up the next step is to consider $u(x,t)$ only at the mesh junction points as in equation L5.1. The parabolic LPCM

$$u(x,t) = u(ih, jl) = u_{i,j} \qquad \text{L5.1}$$

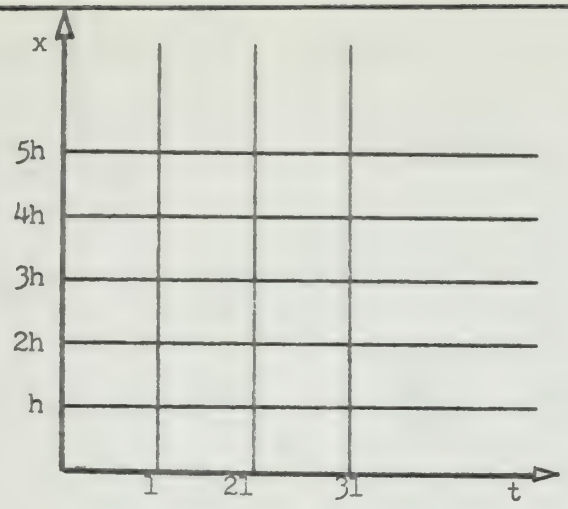


Figure L5.1 - TIME-SPACE MESH FOR NUMERICAL SOLUTIONS

can be solved by either explicit or implicit methods. Explicit methods use only previous and present values of u, such as $u_{i,j}$, $u_{i,j-1}$, . . ., to compute the future value $u_{i,j+1}$. Implicit methods use previous, present, and future values of u to approximate the derivatives at the present point (ih, jl) which are then used to refine the present value of u. Both methods are applicable to the LPCM, but only explicit methods will be discussed here. It is expected that explicit methods would be adequate for solving most cases of the LPCM, but if not, then implicit methods (B2.4 - Numerical Solution Techniques) could be employed. Explicit methods are generally easy to implement and rapid to execute but are relatively unstable compared to implicit methods.

Most finite difference approximations are derived from a Taylor Series expansion of u about the value $u_{i,j}$. Only as many terms in the series are retained as necessary for an accurate solution. A Taylor Series expansion in t with only the first order terms retained

is presented in equation L5.2. Similarly, Taylor Series expansions in x with up to the second order terms retained are presented in equations L5.3 and L5.4.

$$u_{i,j+1} \approx u_{i,j} + \left.\frac{\partial u}{\partial t}\right|_{i,j} 1 \qquad \text{L5.2}$$

$$u_{i-1,j} \approx u_{i,j} - \left.\frac{\partial u}{\partial x}\right|_{i,j} h + \left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} h^2/2 \qquad \text{L5.3}$$

$$u_{i+1,j} \approx u_{i,j} + \left.\frac{\partial u}{\partial x}\right|_{i,j} h + \left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} h^2/2 \qquad \text{L5.4}$$

L5.2 APPLICATION OF EXPLICIT METHODS TO THE LPCM

The basic idea is to use stepwise expressions for u and its derivatives in the LPCM equation, here presented in expanded form is L5.5. In that case the above expansions must be solved for the

$$P_1(x)\frac{\partial^2 u}{\partial x^2} + P_3(x)\frac{\partial u}{\partial x} + P_4(x)u = \frac{\partial u}{\partial t} \qquad \text{L5.5}$$

approximated derivates of u in terms of the previous and present values of u. These solutions will depend upon how many terms of the expansion are used. For the above expansions the approximated values of u and its derivatives are given by equations L5.6 through L5.9.

$$u = u_{i,j} \qquad \text{L5.6}$$

$$\left.\frac{\partial u}{\partial x}\right|_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{h} \qquad \text{L5.7}$$

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \qquad \text{L5.8}$$

$$\left.\frac{\partial u}{\partial t}\right|_{i,j} = \frac{u_{i,j} - u_{i,j-1}}{l} \qquad \text{L5.9}$$

Substituting these approximate relations into the LPCM equation and then solving for $u_{i+1,j}$ gives the recursion relation L5.10 for the LPCM, where the polynomial coefficients are evaluated at x = ih.

$$u_{i+1,j} = (1 - A_i - B_i + C_i)u_{i,j} - A_i u_{i-1,j} - C_i u_{i,j-1} \qquad \text{L5.10}$$

Where: $A_i = 1 - P_3 h/P_1$

$B_i = P_4 h^2/P_1$

$C_i = h^2/(P_1 l)$

$P_i(x)$ are defined in equations L1.30 through L1.33

Using L5.10 and the previously derived equations a numerical iteration scheme can be set up for solving the LPCM along the mesh.

L5.3 BRIEF SUMMARY OF SECTION 3(L)

Section 3(L) concentrates on the Linear Polynomial-Coefficient Model (LPCM) which is derived in Section 2 (M) to represent the transient behavior of a binary plate distillation column. Chapter L1 presents an integral equation procedure for analytical solution of the LPCM in general using Appendices A1, A2, and A3. Chapter L2 applies the solution technique to a reduced form of the LPCM having one spatially varying coefficient and one constant coefficient. A suggested scheme

for a computer program PLPBV to evaluate the solution is presented using Appendices A5 and A6. Chapter L3 evaluates the LPCM for several cases from the steady-state representation of an example column. Chapter L4 solves analytically and evaluates numerically using Appendix A4, four simplified examples of the LPCM: two cases of the best equation and two cases of the Taylor Diffusion Model. The analytical solution steps for the simplified examples are then related to the analytical steps of the integral equation technique of Chapter L1. Chapter L5 discusses briefly several possible numerical methods for solving the LPCM and derives the detailed recursion relations to solve the LPCM by an explicit numerical method.

SECTION 4

SUMMARY AND CONCLUSION (S)

S1 SUMMARY AND CONCLUSIONS

S2 AREAS FOR FURTHER STUDY

" THE PURPOSE OF COMPUTING IS INSIGHT, NOT NUMBERS" — R. W. HAMMING (H-19)

THE CENTRAL PURPOSE OF THIS THESIS IS THE DEVELOPMENT, PRESENTATION, SUGGESTED SOLUTION TECHNIQUE, AND EVALUATION OF THE LINEAR POLYNOMIAL-COEFFICIENT MODEL (LPCM) OF THE DYNAMIC BEHAVIOR OF A BINARY PLATE DISTILLATION COLUMN. THIS SECTION SUMMARIZES THE MAJOR ARGUMENTS PRESENTED IN THIS THESIS RELATING TO THE LPCM AND EMPHASIZES A LARGE NUMBER OF AREAS FOR FURTHER STUDY USING THE LPCM AND THE INTEGRAL EQUATION SOLUTION TECHNIQUE PRESENTED IN THIS THESIS.

CHAPTER S1.

SUMMARY AND CONCLUSIONS

This thesis is summarized in the format of the Chapter and Appendix Relationship Diagram presented in Chapter C2.

S1.1 THE MAIN READING PATH OF CHAPTER C2

Starting from the basic principles of distillation this thesis develops a discrete-plate dynamic model for the composition behavior of a binary plate distillation column. The fact that discrete models characteristically have large solution times leads to the search for a faster model and to the investigation of a continuous-spatial dynamic model derived by treating the plate number in the discrete model as a continuous variable. An investigation of possible solution techniques for the continuous-spatial model leads to the conclusion that for any hope of an analytical solution, the nonlinear continuous-spatial model must be linearized. The representation of the spatial coefficients of the linearized continuous model by general n-th degree polynomials defines the Linear Polynomial-Coefficient Model (LPCM).

The basic equation of the LPCM is presented here as equation S1.1.

$$\frac{\partial^2}{\partial x^2}\left[P_1(x)u\right] + \frac{\partial}{\partial x}\left[P_2(x)u\right] = \frac{\partial u}{\partial t} \qquad \text{S1.1}$$

Where: $P_1(x)$ and $P_2(x)$ are polynomials in x.

Two-point boundary conditions and step initial conditions are specified for u and u_x.

The steady-state solution $u_s(x)$ of the LPCM is obtained by solving the two-point boundary value problem. The transient solution is derived

by converting the spatial ordinary differential eigenvalue problem resulting from separation of variables to a Liouville Normal-Form equation and further transforming to a homogeneous Fredholm II integral equation. The solutions of the integral equation then define the eigenvalues K_i and the eigenfunctions $X_i(x)$. An eigenfunction expansion to meet the initial condition then defines the eigenfunction constants C_i. The total solution to the LPCM is then given by equation S1.2.

$$u(x,t) = u_s(x) + \sum_{i=1}^{n} C_i X_i(x) \exp(-K_i{}^2 t) \qquad \text{S1.2}$$

The integral equation solution technique used to develop equation S1.2 is described in detail by applying it to a first-degree polynomial model (PLPBV) and by suggesting the type of computer program which must be used to evaluate the solution. The individual steps in the solution technique are described analytically by applying the transformation relations to PLPBV and are described numerically by a flowchart of the necessary computation steps and by a very basic Fortran IV digital computer subroutine showing some of the details of the computation steps. Preliminary tests with the PLPBV program suggest that it may be possible to generate complete column solutions in less than one minute for 20 spatial points and 9 time points.

The complete model of a binary plate distillation column using the LPCM consists of two equations of the form of S1.1 and their corresponding two-point boundary conditions. The steps necessary to derive the LPCM for general distillation columns are presented. The details of these steps are then applied, for a second degree model, to a

5-plate and an 11-plate column and the resulting models are presented as examples.

Four simplified versions of the LPCM in the form of the heat equation and the Taylor Diffusion Model are defined as simplified versions of the LPCM. These models are then solved analytically, a computer program used to sum the series is developed, and the solutions are presented graphically and numerically. The standard analytical solution methods for the simplified models are then compared to the general solution technique for the LPCM.

There are a large number of numerical methods which can be applied to any particular distillation column model. Several possible numerical methods for solving the LPCM are discussed, and the detailed recursion relations to solve the LPCM by an explicit numerical method are derived.

The thesis is summarized briefly, and a discussion of a large number of areas for further study is presented.

S1.2 THE AREAS OF OVERALL PERTINENCE OF CHAPTER C2

A bibliography containing 352 references of which 202 pertain to distillation column dynamics and control is presented. These references are then related to four major areas pertinent to the thesis. Some

1. General Theory of Distillation
2. Distillation Column Dynamics
3. Distillation Column Control
4. Mathematics and Computation

general notes, descriptions, and comments pertaining to most of the references are included.

Several opinions on the philosophical aspects of observing reality as related to modeling a distillation column and on the desire to achieve profit as related to the cost of separation of components are presented.

CHAPTER S2

AREAS FOR FURTHER STUDY

This chapter presents,in the form of suggestions, a list of possible topics for further study or areas for further research in the order in which they are encountered by following the main reading path of Chapter C2. It must be emphasized that the LPCM and the integral equation solution technique are suggested by this thesis to be valuable tools for modeling distillation columns, but the validation of this suggestion can only come from further study.

S2.1 SECTION M

1. Using the general discrete equations developed from considering all four (or part) mass balances per plate, develop continuous-spatial models and then LPCM models for the general binary plate column.
2. Investigate other methods of converting discrete models to continuous models which may give continuous models of greater accuracy.
3. Investigate analog computer solution techniques for the CSE and the nonlinear polynomial-class CSE.
4. Find in the literature or develop transformations applicable to the CSE.
5. Apply the Fixed Point Theorem to the CSE,
   a. Show that the CSE is a contraction mapping,
   b. Investigate techniques for finding the fixed point for the CSE.
6. Investigate solution techniques for polynomial-class partial differential equations to see if nonlinear approximated CSE's are more easily solved and less accurate than the general CSE.

7. Investigate the validity and accuracy of models linearized about operating points other than the initial steady-state.

S2.2 SECTION L

8. Investigate the validity of the LPCM as a distillation column model using programs developed and based upon the integral equation solution technique of this thesis.

   a. Complete PLPBV including all special cases.

   b. Develop main modeling program to start from the equilibrium curve and the column physical characteristics and to end up with complete LPCM and solutions using PLPBV.

9. Develop the digital computer programs for the second-degree (and higher) versions of the LPCM and use them to compute column solutions.

10. Develop numerical solution program for the LPCM and compare solution time with the analytical solution programs.

11. Extend the step solution capability of the LPCM to approximate the response to any arbitrary input function of time.

12. Investigate the relative magnitudes of the eigenvalues for several variations of the LPCM in the interest of seeing how many are really necessary to completely characterize column behavior.

13. Apply separable kernel solution procedure to the integral equation resulting from the LPCM and evaluate the accuracy.

14. Investigate in detail the properties of the function M(z) for several variations of the LPCM.

15. Apply the integral equation solution technique to the two-point steady-state boundary-value problem and combine with the transient portion.

16. Develop an LPCM modeling technique for the case when the relative volatility is not constant.

17. Develop an LPCM modeling technique for the case when the Murphree plate efficiencies vary and are not necessarily unity.

18. Investigate in detail the symmetry and continuity properties of the integral equation kernel $K(z,s)$ for various functions $M(z)$.

19. Investigate implicit numerical methods for solving the LPCM and compare solution times to the analytical methods.

20. Investigate the possibilities for partially analytical - partially numerical solutions to the LPCM (hybrid solutions).

S2.3 EXTENSIONS

21. Develop distillation column control schemes particularly suited to using the LPCM.

22. Investigate the possibilities for partially discrete - partially continuous models for distillation columns (hybrid models).

23. Extend the application of the LPCM techniques to packed columns.

24. Extend the application of the LPCM to continuous models of multi-component distillation columns.

25. Combine spatial LPCM and time LPCM solution techniques to solve partial differential two-point boundary-value problems in which the partial differential equation is second order in both time and space. The result of the application of separation of variables will be a spatial LPCM and a time LPCM.

SECTION 5

APPENDICES (A)

"MATHEMATICS POSSESSES NOT ONLY TRUTH, BUT SUPREME BEAUTY — A BEAUTY COLD AND AUSTERE, LIKE THAT OF SCULPTURE, • • • SUBLIMELY PURE, AND CAPABLE OF A STERN PERFECTION SUCH AS ONLY THE GREATEST ART CAN SHOW." — BERTRAND RUSSELL

APPENDIX A1

CONVERSION OF A LIOUVILLE NORMAL-FORM EQUATION TO A FREDHOLM II - INTEGRAL EQUATION

This appendix presents the intermediate steps necessary to the conversion of the Liouville Normal-Form equation (B-14) and its boundary conditions to a Fredholm II - Integral Equation (L-8,H-13). The conversion proceeds via integration of equation A1.1 and application of boundary conditions A1.2, A1.3, and A1.4 to integral equation of the form of A1.5.

$$\frac{d^2W}{dz^2} - [M(z)-\lambda]W = 0 \qquad \text{A1.1}$$

$$D_{11}W(c) + D_{12}W(c) = 0 \qquad \text{A1.2}$$

$$D_{21}W(o) + D_{22}W(o) = 0 \qquad \text{A1.3}$$

$$D_{11}D_{22} - D_{12}D_{21} \neq 0 \qquad \text{A1.4}$$

$$W(z) = \int_o^c K(z,s)W(s)ds \qquad \text{A1.5}$$

Integrating A1.1 from 0 to Z twice and making a change of variable in one of the integrals yields A1.6. Application of the

$$W(z) = \int_o^z [M(z-s)-\lambda]W(s)ds + \overset{o}{W}(o)z + W(o) \qquad \text{A1.6}$$

second boundary condition A1.3 to A1.6 then gives A1.7. The

$$W(z) = \int_o^z [M(z-s)-\lambda]W(s)ds + \left[1-\frac{D_{21}}{D_{22}}z\right]W(o) \qquad \text{A1.7}$$

remainder of the conversion procedure consists of determining

the constant W(0) and placing the resulting equations in integral equation form.

The first step in evaluating W(0) is to integrate equation A1.1 from Z to C, giving equation A1.8. Evaluation of A1.8 at Z = 0

$$\overset{o}{W}(c) = \overset{o}{W}(z) + \int_z^c [M(z)-\lambda]W(z)dz \qquad \text{A1.8}$$

and of A1.7 at Z = C gives A1.9 and A1.10. Placing the boundary

$$\overset{o}{W}(c) = \overset{o}{W}(o) + \int_o^c [M(z)-\lambda]W(z)dz \qquad \text{A1.9}$$

$$W(c) = \int_o^c [M(c-s)-\lambda]W(s)ds + \left[1 - \frac{D_{21}}{D_{22}} c\right]W(o) \qquad \text{A1.10}$$

conditions in the form of A1.11 and A1.12, substituting them into A1.9 and A1.10, and equating them gives A1.13, an equation solely in terms of W(0).

$$W(c) = -\frac{D_{12}}{D_{11}} \overset{o}{W}(c) \qquad \text{A1.11}$$

$$\overset{o}{W}(o) = -\frac{D_{21}}{D_{22}} W(o) \qquad \text{A1.12}$$

$$\int_o^c [M(c-s)-\lambda]W(s)ds + \left[1 - \frac{D_{21}}{D_{22}} c\right]W(o)$$

$$= -\frac{D_{12}}{D_{11}} \left[-\frac{D_{21}}{D_{22}} W(o) + \int_o^c [M(z)-\lambda]W(z)dz\right] \qquad \text{A1.13}$$

Solving for W(0) gives A1.14 and A1.15.

$$W(o) = \frac{1}{C} \int_o^c \left[\left(M(c-s) + \frac{D_{12}}{D_{11}} M(s)\right) - \left(1+\frac{D_{12}}{D_{11}}\right)\lambda\right]$$

$$W(s)ds \qquad \text{A1.14}$$

$$C_o = \frac{D_{12}D_{21}}{D_{11}D_{22}} + \frac{D_{21}}{D_{22}} - 1 \neq 0 \qquad \text{A1.15}$$

If equation A1.14 for W(0) is now substituted back into equation A1.7, then equation A1.16 is an integral equation in W(z). This equation A1.16, however, is not yet in the desired form of A1.5.

$$W(z) = \int_o^z \left[M(z-s)-\lambda\right] W(s)ds + \frac{1}{C_o}\left(1-\frac{D_{21}}{D_{22}}z\right)$$

$$\int_o^c \left[\left(M(c-s) + \frac{D_{12}}{D_{11}}M(s)\right) - \left(1+\frac{D_{12}}{D_{11}}\right)\lambda\right]$$

$$W(s)ds \qquad \text{A1.16}$$

If the kernel function K(z,s) is expressed as the sum in equations A1.17, A1.18, A1.19, and A1.20, then the conversion to the integral equation is complete.

$$K(z,s) = K_1(z,s) + K_2(z,s)$$

$$s\leq z \qquad s>z \qquad \text{A1.17}$$

$$K_1(z,s) = M(z-s) + \frac{1}{C_1}(D_{22}-D_{21}z)$$

$$(D_{11}M(c-s)+C_{12}M(s))$$

$$-\lambda\left[1 + \frac{1}{C_1}(D_{22}-D_{21}z)(D_{11}+D_{12})\right] \qquad \text{A1.18}$$

$$K_2(z,s) = \frac{1}{C_1}(D_{22}-D_{21}z)\left[D_{11}M(c-s)+D_{12}M(s)\right.$$

$$\left.-(D_{11}+D_{12})\lambda\right] \qquad \text{A1.19}$$

$$C_1 = D_{11}D_{22}C_o = D_{12}D_{21} - D_{11}D_{22} + D_{11}D_{21} \qquad \text{A1.20}$$

Thus, the complete integral equation representation of the Liouville Normal-Form equation is summarized in equations A1.20 through A1.24.

$$W(z) = \int_o^c K(z,s)W(s)ds \qquad \text{A1.21}$$

$$K(z,s) = K_1(z,s) + K_2(z,s) \qquad \text{A1.22}$$

$$K_1(z,s) = M(z-s) - \lambda + K_2(z,s) \quad s \leq z \qquad \text{A1.23}$$

$$K_2(z,s) = \frac{1}{C_1}(D_{22}-D_{21}z)\left[D_{11}M(c-s)+D_{12}M(s) - (D_{11}+D_{12})\lambda\right] \quad s \geq z \qquad \text{A1.24}$$

Now, the kernel given in A1.22 must have two properties in order for solution procedures to be applied. It must be continuous at $s = z$ and it must be symmetric. The continuity aspect implies that A1.23 can now be written as A1.25 and A1.26. In this case a new function

$$K_1(z,s) = M(z-s) - M(0) + K_2(z,s) \qquad \text{A1.25}$$

$$K_1(z,s) = \lambda K_3(z,s) \qquad \text{A1.26}$$

$K_3(z,s)$ has been introduced, where $K_2(z,s)$ is given by A1.27 and A1.28. Utilizing once again the continuity requirement and the

$$K_2(z,s) = -M(z,s) + M(0) + \lambda K_3(z,s) \qquad \text{A1.27}$$

$$K_2(z,s) = \lambda K_4(z,s) \qquad \text{A1.28}$$

definition of $K_4(z,s)$ given in A1.28, then $K_4(z,s)$ can be written in terms of $K_3(z,s)$ as in equation A1.29. The remaining kernel

$$K_4(z,s) = 1 - \frac{M(z-s)}{M(0)} + K_3(z,s) \qquad \text{A1.29}$$

Where: $M(0) \neq 0$

function $K_3(z,s)$ can then be expressed as in equation A1.30, and a general test for symmetry can be given by equation A1.31.

$$K_3(z,s) = \frac{M(z,s)}{M(0)} - 1 + \frac{1}{C_1}\,(D_{22} - D_{21}z) \cdot \frac{\left[D_{11}M(c-s) + D_{12}M(s) - (D_{11} + D_{12})\right]}{M(0)} \qquad \text{A1.30}$$

$$C_1\left[M(z-s) - M(0)\right] + (D_{22} - D_{21}z)\left[D_{11}M(c-s) + D_{12}M(s) - M(0)\,(D_{11} + D_{12})\right] \stackrel{?}{=} (D_{22} - D_{21}s)\left[D_{11}M(c-z) + D_{12}M(z) - (D_{11} + D_{12})\,M(0)\right] \qquad \text{A1.31}$$

The summarized equations for the integral equation representation are presented in Figure A1.1.

$$W(z) = \lambda \int_o^c K(z,s)W(s)ds$$

$$K(z,s) = K_3(z,s) + K_4(z,s)$$

$$s \leq z \qquad s \geq z$$

$$K_4(z,s) = 1 - \frac{M(z,s)}{M(0)} + K_3(z,s) \qquad s \geq z$$

$$K_3(z,s) = \frac{M(z-s)}{M(0)} - 1 + \frac{1}{C_1}\,(D_{22} - D_{21}z) \cdot \left[\frac{D_{11}M(c-s) + D_{12}M(s)}{M(0)} - (D_{11} + D_{12})\right] \qquad s \leq z$$

Figure A1.1 - THE FREDHOLM II - HOMOGENEOUS INTEGRAL EQUATION

APPENDIX A2

SOLUTION OF A HOMOGENEOUS FREDHOLM II-INTEGRAL EQUATION WITH A SEPARABLE KERNEL

This appendix presents the developments necessary for finding the solution to a separable kernel integral equation. The integral equation A2.1 and separable kernel A2.2 are combined and a matrix solution technique is developed. The technique to be presented is standard throughout the literature when it is recognized that the following terms are equivalent to "separable kernel" A2.2.

1. Separable Kernel (H-13) (L-8)
2. Degenerate Kernel (P-4) (G-7)
3. Kernel of Finite Rank (S-11)
4. Pincherle-Goursat Kernels (T-3)
5. Riesz-Schauder Equations (M-6)

$$W(z) = \lambda \int_o^c K(z,s)W(s)ds \qquad \text{A2.1}$$

$$K(z,s) = \sum_{i=1}^{m} a_i(z)b_i(s) \qquad \text{A2.2}$$

If A2.2 is substituted into A2.1 and the integral and summation signs interchanged, then equation A2.3 results. It can be seen that the integrated terms depend only upon S and are therefore constants A2.4 after integration. Thus, the solution to A2.1 can be expressed

$$W(z) = \lambda_i \sum_{i=1}^{m} a_i(z) \int_o^c b_i(s)W(s)ds \qquad \text{A2.3}$$

$$C_i = \int_o^c b_i(s)W(s)ds \qquad \text{A2.4}$$

in terms of the constants C_i as equation A2.5, and the problem now becomes that of finding the C_i.

$$W(z) = \lambda_i \sum_{i=1}^{m} a_i(z) C_i \qquad \text{A2.5}$$

The first step in finding the C_i is the substitution of A2.5 back into A2.4 giving A2.6. The terms involving the integral of $a_i(s)$ and $b_i(s)$ are then recognized as constants A_{ij} of equation A2.7, which can be calculated from the given kernel function A2.2. The resulting equation A2.8 is a system of m simultaneous equations in

$$C_i = \lambda_j \sum_{j=1}^{m} C_j \int_o^c b_i(s) a_j(s) ds \qquad \text{A2.6}$$

$$A_{ij} = \int_o^c b_i(s) a_j(s) ds \qquad \text{A2.7}$$

$$C_i = \lambda_j \sum_{j=1}^{m} A_{ij} C_j \qquad \text{A2.8}$$

the m unknown constants C_i.

Equation A2.8 now represents a matrix eigenvalue problem. This can be seen by expanding A2.8 and writing it in the form of A2.9, where $\sigma = 1/\lambda$. Equation A2.9 can then be written in the form of

$$\begin{bmatrix} \sigma - A_{11} & -A_{12} & \cdots & -A_{1m} \\ -A_{21} & \sigma - A_{22} & \cdots & -A_{2m} \\ \vdots & \vdots & & \vdots \\ -A_{m1} & -A_{m2} & \cdots & \sigma - A_{mm} \end{bmatrix} \begin{bmatrix} C_1 \\ C_2 \\ \vdots \\ C_m \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \qquad \text{A2.9}$$

$$\sigma = \frac{1}{\lambda} \qquad \text{A2.10}$$

A2.11, which is a matrix eigenvalue problem.

$$(\sigma I - A)C = 0 \qquad \text{A2.11}$$

The matrix eigenvalue problem A2.11 must now be solved. The first requirement for solutions to exist is that the determinant of the matrix be zero as in A2.12. This specifies an m^{th} order polynomial in σ which when solved gives the m - real roots or eigenvalues σ_i; i = 1,m. For each of these σ_i there must exist an eigenvector E_i such that A2.13 is satisfied.

$$\det (\sigma I - A) = 0 \qquad \text{A2.12}$$

$$(\sigma_i I - A)E_i = 0 \qquad \text{A2.13}$$

Once these eigenvalues and eigenvectors are known, the first solution can be expressed by A2.14. It must be emphasized that there are m - solutions $W_i(z)$ to this problem, one for each eigenvalue.

$$\sigma_1 \; ; \quad W_1(z) = \sum_{i=1}^{m} a_i(z) \frac{E_{1i}}{\sigma_1} \qquad \text{A2.14}$$

Thus, the eigenfunction solutions to the equation A2.1 are given in A2.15.

$$W_i(z) = \sum_{j=1}^{m} \lambda_i a_j(z) E_{ij} \qquad \text{A2.15}$$

APPENDIX A3

SOLUTION OF A HOMOGENEOUS FREDHOLM II-INTEGRAL EQUATION BY CONVERSION TO LINEAR ALGEBRAIC EQUATIONS

This appendix presents an approximate solution technique for determining the eigenvalues and eigenfunctions of an integral equation A3.1 by dividing the integration interval into equally spaced increments and changing the integral to an algebraic summation. The

$$W(z) = \lambda \int_0^C K(z,s)W(s)ds \qquad \text{A3.1}$$

integral equation eigenvalue problem is thus changed to a matrix eigenvalue problem. The approximate solution W(z) can then be expressed in terms of the eigenvalues and eigenvectors of the matrix eigenvalue problem. References for this material are: (H-13) (L-8) (P-4) (G-7) (S-11) (T-3) (V-4) (S-14) (D-5) and (M-6).

The first step in this solution technique is to divide the interval $[0,C]$ into n equal parts of length δ as in equation A3.2.

$$\delta = \frac{C}{n} \qquad \text{A3.2}$$

Next, the functions W(z) and K(z,s) can be evaluated along the interval as A3.5 and A3.6 at each of the points given by A3.3 and A3.4.

$$K(i\delta, j\delta) = K_{ij} \quad (i,j = 1, 2, \cdots, n) \qquad \text{A3.3}$$

$$W(i\delta) = W_i \quad (i = 1, 2, \cdots, n) \qquad \text{A3.4}$$

$$z_i = i\delta \quad (i = 1, 2, \cdots, n) \qquad \text{A3.5}$$

$$s_j = j\delta \quad (j = 1, 2, \cdots, n) \qquad \text{A3.6}$$

With these relationships established, the integral in A3.1 is

approximated by a summation over the interval [0,c] represented by the indices [1,n] as in equation A3.7.

$$W_i = \lambda \sum_{j=1}^{n} K_{ij} W_j \delta \qquad \text{A3.7}$$

Equation A3.7 represents a matrix eigenvalue problem similar to equation A2.8 in Appendix A2. This equation A3.7 can be placed in eigenvalue form A3.9 by defining θ as in A3.8, similar to equations A2.9, A2.10, and A2.11 in Appendix A2.

$$\theta = \frac{1}{\lambda \delta} \qquad \text{A3.8}$$

$$(\theta I - A)W = 0 \qquad \text{A3.9}$$

Once the eigenvalues θ_i and eigenvectors E_i for equation A3.9 are found, the approximate solution to equation A3.1 can be expressed as A3.10.

$$W_i(z) = \lambda_i \delta \sum_{j=1}^{n} K(z, j\delta) E_{ij} \qquad \text{A3.10}$$

APPENDIX A4

DIGITAL COMPUTER PROGRAM AND OUTPUT FOR EVALUATION OF PROBLEMS IN CHAPTER L4

This appendix presents a listing of the Fortran IV statements in the program and subroutines used to calculate the numerical values of the four analytical solutions presented in Chapter L4. The numerical results are first listed, then plotted, and finally printed out in matrix form. Tests made with this program showed that in all cases less than ten terms in the series were used for three-decimal-place accuracy.

There are three subroutines used in the program: MXOUT, PLOT, and LOC. Subroutine LOC was taken, less comment cards, directly from reference (I-3), the Scientific Subroutine Package. Subroutines MXOUT and PLOT, used here, represent significantly modified versions of the MXOUT and PLOT subroutines described in reference (I-3). The main program and subroutines are written in Fortran IV, and all runs were compiled and executed using the WATFOR compiler on the IBM 360/65 computer at the M.I.T. Computation Center. The entire program compiles in 5.8 seconds and executes in 5.65 seconds.

```
C PROGRAM TO CALCULATE 4 TRANSIENT RESPONSES,UA1,UA2,UB1,UC1
C PROGRAM TO CALCULATE 4 ANALYTIC SOLUTIONS AS A TEST
      DIMENSION UA(100),UAT(100),UB(100),UC(100)
  100 FORMAT(3X,'X=',3X,'T=',7X,'UAONE=',6X,'UATWO=',6X,
     1'UBONE=',6X,'UCONE=',//)
  102 FORMAT(1X,'UATWO NOT 1 PERCENT ACCURATE,X=',F7.3,
     1'  T=',F7.3)
  103 FORMAT(1X,'UAONE NOT ONE PERCENT ACCURATE,X=',F7.3,
     1'  T=',F7.3)
  104 FORMAT(1X,'UBONE AND UCONE NOT ONE PERCENT ACCURATE,X=',
     1F7.3,'T=',F7.3)
  105 FORMAT(1X,2F5.2,3X,4E12.5)
      PI=3.14159265
      DELTT=0.025
      DELTX=0.1
      MIN=1.0E-07
      A=1.118
      B=PI*PI*A*A
      BN=0.25*B
      WRITE(6,100)
C THIS SECTION IS TO SET UP OUTPUT PLOTS AT 0.1 INTERVALS
C IN X.
      XP=0.0
      DO 200 I=1,10
      XP=XP+DELTX
      UA(I)=XP
      UAT(I)=XP
      UB(I)=XP
      UC(I)=XP
  200 CONTINUE
      I=11
      T=0.0
      DO 10 J=1,9
      T=T+DELTT
      X=0.0
      DO 20 K=1,10
      X=X+DELTX
C TIME-SPACE GRID IS NOW SET
C STEADY STATE CALCULATIONS
      UASST=X
      UATST=1.0
      AC=1.0/(A*A)
      UBOST=(1.0-EXP(AC*X))/(1.0-EXP(AC))
      UCCST=(1.0-EXP(-AC*X))/(1.0-EXP(-AC))
C TRANSIENT CALCULATIONS
      SN=-1.0
      UAOTR=0.0
      UATTR=0.0
      UBOTR=0.0
      ATB=2.0*EXP((-0.25*T+0.5*X-0.5)*AC)
      ATC=2.0*EXP((-0.25*T+0.5-0.5*X)*AC)
      IAO=0
      IAT=0
```

```
      IBO=0
      IFIN=0
C USE ONLY THE FIRST 400 TERMS OR LESS OF THE SERIES
      DO 30 N=1,400
      IF(IFIN-3)53,54,54
   53 RN=FLOAT(N)
      AN=RN*PI
      IF(IAT)41,41,42
   41 RTN=FLOAT(2*N-1)
      ATN=RTN*PI
      COSN=COS(ATN*X*0.5)
      EXPBN=EXP(-RTN*RTN*T*BN)
      UATT=UATTR
      UATTR=UATTR+(SN*COSN*EXPBN)/(ATN*0.5)
      IF(ABS(UATTR)-MIN)44,44,61
   61 IF(ABS((UATTR-UATT)/UATTR)-0.01)43,43,42
   44 UATTR=0.0
   43 IAT=1
      IFIN=IFIN+1
   42 SINN=SIN(AN*X)
      EXPB=EXP(-RN*RN*T*B)
      IF(IAO)45,45,46
   45 UAO=UAOTR
      UAOTR=UAOTR+(SN*SINN*EXPB)/AN
      IF(ABS(UAOTR)-MIN)48,48,62
   62 IF(ABS((UAOTR-UAO)/UAOTR)-0.01)47,47,46
   48 UAOTR=0.0
   47 IAO=1
      IFIN=IFIN+1
   46 IF(IBO)49,49,50
   49 UBO=UBOTR
      SUMSQ=0.25*AC*AC+AN*AN
      UBOTR=UBOTR+(SN*AN*SINN*EXPB)/SUMSQ
      IF(ABS(UBOTR)-MIN)52,52,63
   63 IF(ABS((UBOTR-UBO)/UBOTR)-0.01)51,51,50
   52 UBOTR=0.0
   51 IBO=1
      IFIN=IFIN+1
   50 SN=-SN
   30 CONTINUE
      IF(IAT)55,55,56
   55 WRITE(6,102)X,T
   56 IF(IAO)57,57,58
   57 WRITE(6,103)X,T
   58 IF(IBO)59,59,54
   59 WRITE(6,104)X,T
   54 ATR=2.0*UAOTR
      UAONE=UAOST+ATR
      ATTR=2.0*UATTR
      UATWO=UATST+ATTR
      BTR=ATB*UBOTR
      CTR=ATC*UBOTR
      UBONE=UBOST+BTR
      UCONE=UCOST+CTR
C SAVE VALUES FOR PLOTTING
```

```
      UA(I)=UAONE
      UAT(I)=UATWO
      UB(I)=UBONE
      UC(I)=UCONE
      I=I+1
      WRITE(6,105)X,T,UAONE,UATWO,UBONE,UCONE
   20 CONTINUE
   10 CONTINUE
C PLOT COMMANDS
C MATRIX PRINTOUT
      NO=1
      MP=10
      NP=10
      MS=0
      LINS=45
      IPOS=65
      ISP=1
      NL=46
      NS=1
      CALL PLOT(NO, UA,NP,MP,NL,NS)
      CALL MXOUT(NO, UA,NP,MP,MS,LINS,IPOS,ISP)
      NO=NO+1
      CALL PLOT(NO,UAT,NP,MP,NL,NS)
      CALL MXOUT(NO,UAT,NP,MP,MS,LINS,IPOS,ISP)
      NO=NO+1
      CALL PLOT(NO, UB,NP,MP,NL,NS)
      CALL MXOUT(NO, UB,NP,MP,MS,LINS,IPOS,ISP)
      NO=NO+1
      CALL PLOT(NO, UC,NP,MP,NL,NS)
      CALL MXOUT(NO, UC,NP,MP,MS,LINS,IPOS,ISP)
      CALL EXIT
      END
```

```
      SUBROUTINE PLOT(NO,A,N,M,NL,NS)
C     ********** MICHAEL N. HAYES **********
      DIMENSION OUT(101),YPR(11),IANG(9),A(1)
      INTEGER IDUM/'1'/,IANG/'1','2','3','4','5','6','7',
     1'8','9'/
      INTEGER OUT
C     THESE LIMITED FORMATS ARE FOR 60 SPACE PRINTOUTS FOR
C     THESIS USE.
    1 FORMAT(1H1,28X,7H CHART ,I3,//)
    2 FORMAT(1H ,F8.3,1X,'*',51A1,'*')
    3 FORMAT(1H )
    7 FORMAT(1H ,10X,36H*     *     *     *     *     *     *     *,
     115H     *     *     *)
    8 FORMAT(1HO,8X,11F5.2)
C     NTH IS NUMBER OF SPACES TO BE USED, EITHER 101 OR 51
      NTH=51
      NLL=NL
      IF(NS)16,16,10
   10 DO 15 I=1,N
      DO 14 J=I,N
      IF(A(J)-A(I))14,14,11
   11 L=I-N
      LL=J-N
      DO 12 K=1,M
      L=L+N
      LL=LL+N
      F=A(L)
      A(L)=A(LL)
   12 A(LL)=F
   14 CONTINUE
   15 CONTINUE
   16 IF(NLL)20,18,20
   18 NLL=50
   20 WRITE(6,1)NO
      WRITE(6,7)
      BLANK=0
      XSCAL=(A(N)-A(1))/(FLOAT(NLL-1))
      M1=N+1
      YMAX=-1.0E75
      YMIN=1.0E75
      M2=M*N
      DO 40 J=M1,M2
      IF (A(J) .GT. YMAX) YMAX=A(J)
      IF (A(J) .LT. YMIN) YMIN=A(J)
   40 CONTINUE
      YSCAL=(YMAX-YMIN)/50.0
      XB=A(1)
      L=1
      MY=M-1
      I=1
   45 F=I-1
      XPR=XB+F*XSCAL
      IF(XPR-A(L))50,50,70
   50 DO 55 IX=1,NTH
   55 OUT(IX)=BLANK
```

```
      DO 60 J=1,MY
      LL=L+J*N
      JP=((A(LL)-YMIN)/YSCAL)+1.0
      OUT(JP)=IANG(J)
   60 CONTINUE
C     PROPER FORMAT CARDS MUST BE USED
      WRITE(6,2)XPR,(OUT(IZ),IZ=1,NTH)
      L=L+1
      GO TO 80
   70 WRITE(6,3)
   80 I=I+1
      IF(I-NLL)45,84,86
   84 XPR=A(N)
      GO TO 50
   86 WRITE(6,7)
      YPR(1)=YMIN
      DO 90 KN=1,9
   90 YPR(KN+1)=YPR(KN)+YSCAL*5.0
      YPR(11)=YMAX
      WRITE(6,8)(YPR(IP),IP=1,11)
      RETURN
      END
```

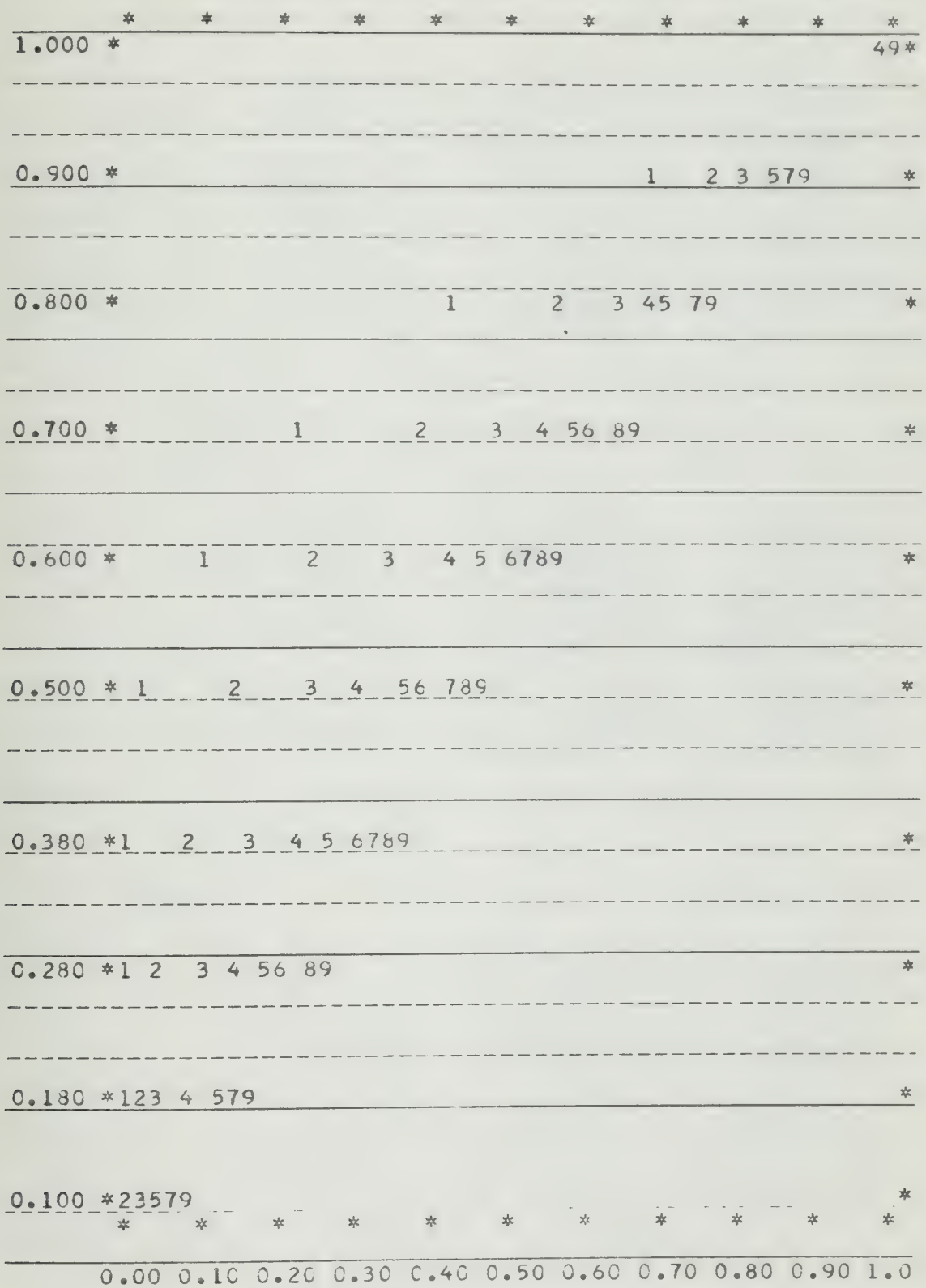
```
      SUBROUTINE MXOUT (ICODE,A,N,M,MS,LINS,IPOS,ISP)
C     ********** MICHAEL N. HAYES **********
      DIMENSION A(1),B(8)
    1 FORMAT(1HO,5X, 7HMATRIX ,I5,6X,I3,5H ROWS,6X,I3,
     18H COLUMNS,/)
    2 FORMAT(12X,8HCOLUMN  ,7(3X,I3,10X))
    3 FORMAT(1H )
    4 FORMAT(1H ,7X,4HROW ,I3,7(E16.6))
    5 FORMAT(1HO,7X,4HROW ,I3,7(E16.6))
    6 FORMAT(1H1)
    7 FORMAT(16X,13HSTORAGE MODE ,I1,7X,7HGROUP ,I2,/)
      WRITE(6,6)
      J=1
      NEND=IPOS/16-1
      LEND=(LINS/ISP)-2
      IPAGE=1
   10 LSTRT=1
   20 WRITE(6,1)ICODE,N,M
      WRITE(6,7)MS,IPAGE
      JNT=J+NEND-1
      IPAGE=IPAGE+1
   31 IF(JNT-M)33,33,32
   32 JNT=M
   33 CONTINUE
      WRITE(6,2)(JCUR,JCUR=J,JNT)
      IF(ISP-1)35,35,40
   35 WRITE(6,3)
   40 LTEND=LSTRT+LEND-1
      DO 80 L=LSTRT,LTEND
      DO 55 K=1,NEND
      KK=K
      JT=J+K-1
      CALL LOC(L,JT,IJNT,N,M,MS)
      B(K)=0.0
      IF(IJNT)50,50,45
   45 B(K)=A(IJNT)
   50 CONTINUE
      IF(JT-M)55,60,60
   55 CONTINUE
   60 IF(ISP-1)65,65,70
   65 WRITE(6,4)L,(B(JW),JW=1,KK)
      GO TO 75
   70 WRITE(6,5)L,(B(JW),JW=1,KK)
   75 IF(N-L)85,85,80
   80 CONTINUE
      LSTRT=LSTRT+LEND
      GO TO 20
   85 IF(JT-M)90,95,95
   90 J=JT+1
      GO TO 10
   95 RETURN
      END
```

```
      SUBROUTINE LOC(I,J,IR,N,M,MS)
C     ***********************************************
      IX=I
      JX=J
      IF(MS-1) 10,20,30
   10 IRX=N*(JX-1)+IX
      GO TO 36
   20 IF(IX-JX) 22,24,24
   22 IRX=IX+(JX*JX-JX)/2
      GO TO 36
   24 IRX=JX+(IX*IX-IX)/2
      GO TO 36
   30 IRX=0
      IF(IX-JX) 36,32,36
   32 IRX=IX
   36 IR=IRX
      RETURN
      END
```

X=	T=	UAONE=	UATWO=	UBONE=	UCONE=
0.10	0.02	0.30595E-03	0.37324E-03	0.21213E-03	0.43643E-03
0.20	0.02	0.13734E-02	0.35691E-02	0.99301E-03	0.18837E-02
0.30	0.02	0.50529E-02	0.49801E-02	0.38026E-02	0.66583E-02
0.40	0.02	0.16391E-01	0.16605E-01	0.12842E-01	0.20754E-01
0.50	0.02	0.32329E-01	0.45695E-01	0.26402E-01	0.39390E-01
0.60	0.02	0.10959E 00	0.10548E 00	0.93069E-01	0.12817E 00
0.70	0.02	0.22939E 00	0.22987E 00	0.20286E 00	0.25789E 00
0.80	0.02	0.42370E 00	0.42378E 00	0.39023E 00	0.45795E 00
0.90	0.02	0.68921E 00	0.68916E 00	0.66130E 00	0.71638E 00
1.00	0.02	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.05	0.90371E-02	0.12726E-01	0.62542E-02	0.12850E-01
0.20	0.05	0.22954E-01	0.24391E-01	0.16539E-01	0.31367E-01
0.30	0.05	0.47477E-01	0.48038E-01	0.35616E-01	0.62355E-01
0.40	0.05	0.89609E-01	0.89781E-01	0.69999E-01	0.11313E 00
0.50	0.05	0.15644E 00	0.15724E 00	0.12727E 00	0.18987E 00
0.60	0.05	0.25787E 00	0.25780E 00	0.21850E 00	0.30091E 00
0.70	0.05	0.39612E 00	0.39612E 00	0.34967E 00	0.44453E 00
0.80	0.05	0.57160E 00	0.57160E 00	0.52579E 00	0.61703E 00
0.90	0.05	0.77730E 00	0.77729E 00	0.74534E 00	0.80742E 00
1.00	0.05	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.07	0.26589E-01	0.48732E-01	0.18346E-01	0.37694E-01
0.20	0.07	0.59082E-01	0.70247E-01	0.42445E-01	0.80500E-01
0.30	0.07	0.10328E 00	0.10809E 00	0.77266E-01	0.13527E 00
0.40	0.07	0.16462E 00	0.16707E 00	0.12827E 00	0.20731E 00
0.50	0.07	0.24762E 00	0.24873E 00	0.20100E 00	0.29986E 00
0.60	0.07	0.35538E 00	0.35581E 00	0.30057E 00	0.41393E 00
0.70	0.07	0.48832E 00	0.48849E 00	0.43045E 00	0.54721E 00
0.80	0.07	0.64413E 00	0.64419E 00	0.59193E 00	0.69464E 00
0.90	0.07	0.81735E 00	0.81737E 00	0.78334E 00	0.84859E 00
1.00	0.07	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.10	0.44050E-01	0.99654E-01	0.30318E-01	0.62289E-01
0.20	0.10	0.93196E-01	0.12598E 00	0.66789E-01	0.12667E 00
0.30	0.10	0.15218E 00	0.17074E 00	0.11359E 00	0.19886E 00
0.40	0.10	0.22501E 00	0.23523E 00	0.17496E 00	0.28276E 00
0.50	0.10	0.31459E 00	0.31999E 00	0.25489E 00	0.38026E 00
0.60	0.10	0.42232E 00	0.42507E 00	0.35664E 00	0.49115E 00
0.70	0.10	0.54782E 00	0.54916E 00	0.48231E 00	0.61315E 00
0.80	0.10	0.68884E 00	0.68945E 00	0.63249E 00	0.74225E 00
0.90	0.10	0.84136E 00	0.84159E 00	0.80602E 00	0.87315E 00
1.00	0.10	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.12	0.58303E-01	0.15648E 00	0.40041E-01	0.82266E-01
0.20	0.12	0.12058E 00	0.18421E 00	0.86230E-01	0.16354E 00
0.30	0.12	0.19044E 00	0.23051E 00	0.14186E 00	0.24837E 00
0.40	0.12	0.27086E 00	0.29536E 00	0.21022E 00	0.33975E 00
0.50	0.12	0.36380E 00	0.37836E 00	0.29428E 00	0.43903E 00
0.60	0.12	0.47007E 00	0.47845E 00	0.39643E 00	0.54594E 00
0.70	0.12	0.58918E 00	0.59381E 00	0.51818E 00	0.65874E 00
0.80	0.12	0.71931E 00	0.72171E 00	0.66000E 00	0.77452E 00
0.90	0.12	0.85752E 00	0.85853E 00	0.82120E 00	0.88960E 00
1.00	0.12	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.15	0.69195E-01	0.21407E 00	0.47435E-01	0.97457E-01

0.20	0.15	0.14137E 00	0.24144E 00	0.10092E 00	0.19141E 00
0.30	0.15	0.21924E 00	0.28673E 00	0.16304E 00	0.28544E 00
0.40	0.15	0.30495E 00	0.34939E 00	0.23632E 00	0.38193E 00
0.50	0.15	0.39994E 00	0.42846E 00	0.32308E 00	0.48199E 00
0.60	0.15	0.50473E 00	0.52251E 00	0.42516E 00	0.58551E 00
0.70	0.15	0.61887E 00	0.62952E 00	0.54380E 00	0.69132E 00
0.80	0.15	0.74100E 00	0.74692E 00	0.67948E 00	0.79739E 00
0.90	0.15	0.86897E 00	0.87159E 00	0.83190E 00	0.90120E 00
1.00	0.15	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.17	0.77320E-01	0.26988E 00	0.52922E-01	0.10873E 00
0.20	0.17	0.15685E 00	0.29607E 00	0.11180E 00	0.21204E 00
0.30	0.17	0.24059E 00	0.33922E 00	0.17866E 00	0.31279E 00
0.40	0.17	0.33013E 00	0.39853E 00	0.25549E 00	0.41291E 00
0.50	0.17	0.42650E 00	0.47286E 00	0.34412E 00	0.51339E 00
0.60	0.17	0.53006E 00	0.56061E 00	0.44606E 00	0.61429E 00
0.70	0.17	0.64048E 00	0.65979E 00	0.56236E 00	0.71491E 00
0.80	0.17	0.75674E 00	0.76798E 00	0.69355E 00	0.81390E 00
0.90	0.17	0.87725E 00	0.88240E 00	0.83961E 00	0.90955E 00
1.00	0.17	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.20	0.83324E-01	0.32281E 00	0.56958E-01	0.11702E 00
0.20	0.20	0.16828E 00	0.34748E 00	0.11980E 00	0.22720E 00
0.30	0.20	0.25633E 00	0.38803E 00	0.19012E 00	0.33285E 00
0.40	0.20	0.34866E 00	0.44360E 00	0.26953E 00	0.43560E 00
0.50	0.20	0.44600E 00	0.51297E 00	0.35951E 00	0.53634E 00
0.60	0.20	0.54864E 00	0.59455E 00	0.46131E 00	0.63529E 00
0.70	0.20	0.65630E 00	0.68643E 00	0.57587E 00	0.73209E 00
0.80	0.20	0.76825E 00	0.78634E 00	0.70378E 00	0.82590E 00
0.90	0.20	0.88330E 00	0.89176E 00	0.84521E 00	0.91561E 00
1.00	0.20	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01
0.10	0.22	0.87745E-01	0.37243E 00	0.59914E-01	0.12310E 00
0.20	0.22	0.17669E 00	0.39549E 00	0.12565E 00	0.23831E 00
0.30	0.22	0.26791E 00	0.43333E 00	0.19851E 00	0.34754E 00
0.40	0.22	0.36228E 00	0.48510E 00	0.27980E 00	0.45220E 00
0.50	0.22	0.46033E 00	0.54960E 00	0.37075E 00	0.55311E 00
0.60	0.22	0.56227E 00	0.62531E 00	0.47245E 00	0.65063E 00
0.70	0.22	0.66790E 00	0.71039E 00	0.58574E 00	0.74463E 00
0.80	0.22	0.77668E 00	0.80276E 00	0.71124E 00	0.83466E 00
0.90	0.22	0.88774E 00	0.90011E 00	0.84930E 00	0.92004E 00
1.00	0.22	0.10000E 01	0.10000E 01	0.10000E 01	0.10000E 01

CHART 1


1.000 * 49*
0.900 * 1 2 3 579 *
0.800 * 1 2 3 45 79 *
0.700 * 1 2 3 4 56 89 *
0.600 * 1 2 3 4 5 6789 *
0.500 * 1 2 3 4 56 789 *
0.380 *1 2 3 4 5 6789 *
0.280 *1 2 3 4 56 89 *
0.180 *123 4 579 *
0.100 *23579 *
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.0

MATRIX 1 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 1

	COLUMN	1	2	3
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.900000E 00	0.689206E 00	0.777299E 00
ROW	3	0.800000E 00	0.423696E 00	0.571601E 00
ROW	4	0.700000E 00	0.229394E 00	0.396123E 00
ROW	5	0.600000E 00	0.109590E 00	0.257871E 00
ROW	6	0.500000E 00	0.323286E-01	0.156441E 00
ROW	7	0.400000E 00	0.163907E-01	0.896093E-01
ROW	8	0.300000E 00	0.505292E-02	0.474771E-01
ROW	9	0.200000E 00	0.137341E-02	0.229545E-01
ROW	10	0.100000E 00	0.305951E-03	0.903708E-02

MATRIX 1 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 2

	COLUMN	4	5	6
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.817346E 00	0.841358E 00	0.857519E 00
ROW	3	0.644126E 00	0.688840E 00	0.719308E 00
ROW	4	0.488323E 00	0.547825E 00	0.589176E 00
ROW	5	0.355377E 00	0.422323E 00	0.470072E 00
ROW	6	0.247616E 00	0.314594E 00	0.363798E 00
ROW	7	0.164620E 00	0.225015E 00	0.270856E 00
ROW	8	0.103279E 00	0.152181E 00	0.190444E 00
ROW	9	0.590816E-01	0.931960E-01	0.120577E 00
ROW	10	0.265891E-01	0.440498E-01	0.583032E-01

MATRIX 1 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 3

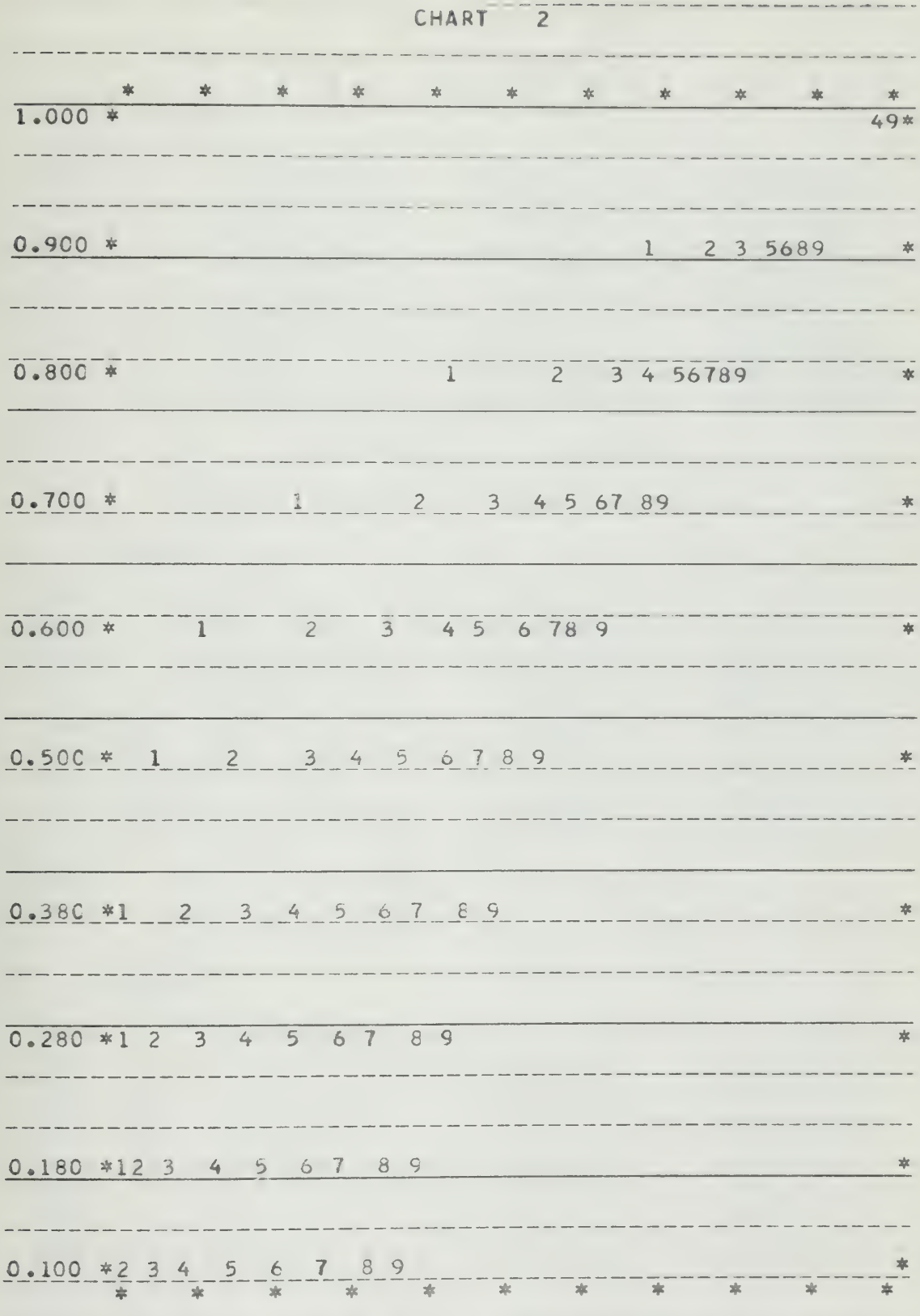
	COLUMN	7	8	9
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.868967E 00	0.877253E 00	0.883305E 00
ROW	3	0.741004E 00	0.756742E 00	0.768246E 00
ROW	4	0.613868E 00	0.640481E 00	0.656300E 00
ROW	5	0.504727E 00	0.530061E 00	0.548636E 00
ROW	6	0.399944E 00	0.426497E 00	0.446003E 00
ROW	7	0.304955E 00	0.330128E 00	0.348656E 00
ROW	8	0.219237E 00	0.240588E 00	0.256331E 00
ROW	9	0.141373E 00	0.156850E 00	0.168277E 00
ROW	10	0.691950E-01	0.773195E-01	0.833238E-01

MATRIX 1 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 4

COLUMN	10
ROW 1	0.100000E 01
ROW 2	0.887740E 00
ROW 3	0.776680E 00
ROW 4	0.667904E 00
ROW 5	0.562272E 00
ROW 6	0.460333E 00
ROW 7	0.362277E 00
ROW 8	0.267913E 00
ROW 9	0.176689E 00
ROW 10	0.877451E-01

CHART 2


1.000 * 49*
0.900 * 1 2 3 5689 *
0.800 * 1 2 3 4 56789 *
0.700 * 1 2 3 4 5 67 89 *
0.600 * 1 2 3 4 5 6 78 9 *
0.500 * 1 2 3 4 5 6 7 8 9 *
0.380 *1 2 3 4 5 6 7 8 9 *
0.280 *1 2 3 4 5 6 7 8 9 *
0.180 *12 3 4 5 6 7 8 9 *
0.100 *2 3 4 5 6 7 8 9 *
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.0

MATRIX 2 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 1

COLUMN	1	2	3
ROW 1	0.100000E 01	0.999999E 00	0.100000E 01
ROW 2	0.900000E 00	0.689158E 00	0.777291E 00
ROW 3	0.800000E 00	0.423778E 00	0.571596E 00
ROW 4	0.700000E 00	0.229871E 00	0.396115E 00
ROW 5	0.600000E 00	0.105476E 00	0.257800E 00
ROW 6	0.500000E 00	0.456947E-01	0.157242E 00
ROW 7	0.400000E 00	0.166054E-01	0.897810E-01
ROW 8	0.300000E 00	0.498009E-02	0.480379E-01
ROW 9	0.200000E 00	0.356913E-02	0.243909E-01
ROW 10	0.100000E 00	0.373244E-03	0.127263E-01

MATRIX 2 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 2

COLUMN	4	5	6
ROW 1	0.100000E 01	0.100000E 01	0.100000E 01
ROW 2	0.817368E 00	0.841594E 00	0.858528E 00
ROW 3	0.644190E 00	0.689454E 00	0.721705E 00
ROW 4	0.488495E 00	0.549163E 00	0.593811E 00
ROW 5	0.355814E 00	0.425069E 00	0.478449E 00
ROW 6	0.248729E 00	0.319994E 00	0.378359E 00
ROW 7	0.167068E 00	0.235234E 00	0.295359E 00
ROW 8	0.108085E 00	0.170740E 00	0.230511E 00
ROW 9	0.702469E-01	0.125980E 00	0.184211E 00
ROW 10	0.487320E-01	0.996541E-01	0.156484E 00

MATRIX 2 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 3

COLUMN	7	8	9
ROW 1	0.100000E 01	0.100000E 01	0.100000E 01
ROW 2	0.871591E 00	0.882398E 00	0.891763E 00
ROW 3	0.746924E 00	0.767981E 00	0.786335E 00
ROW 4	0.629523E 00	0.659794E 00	0.686427E 00
ROW 5	0.522506E 00	0.560613E 00	0.594554E 00
ROW 6	0.428458E 00	0.472858E 00	0.512968E 00
ROW 7	0.349387E 00	0.398534E 00	0.443600E 00
ROW 8	0.286730E 00	0.339217E 00	0.388030E 00
ROW 9	0.241436E 00	0.296071E 00	0.347479E 00
ROW 10	0.214071E 00	0.269883E 00	0.322809E 00

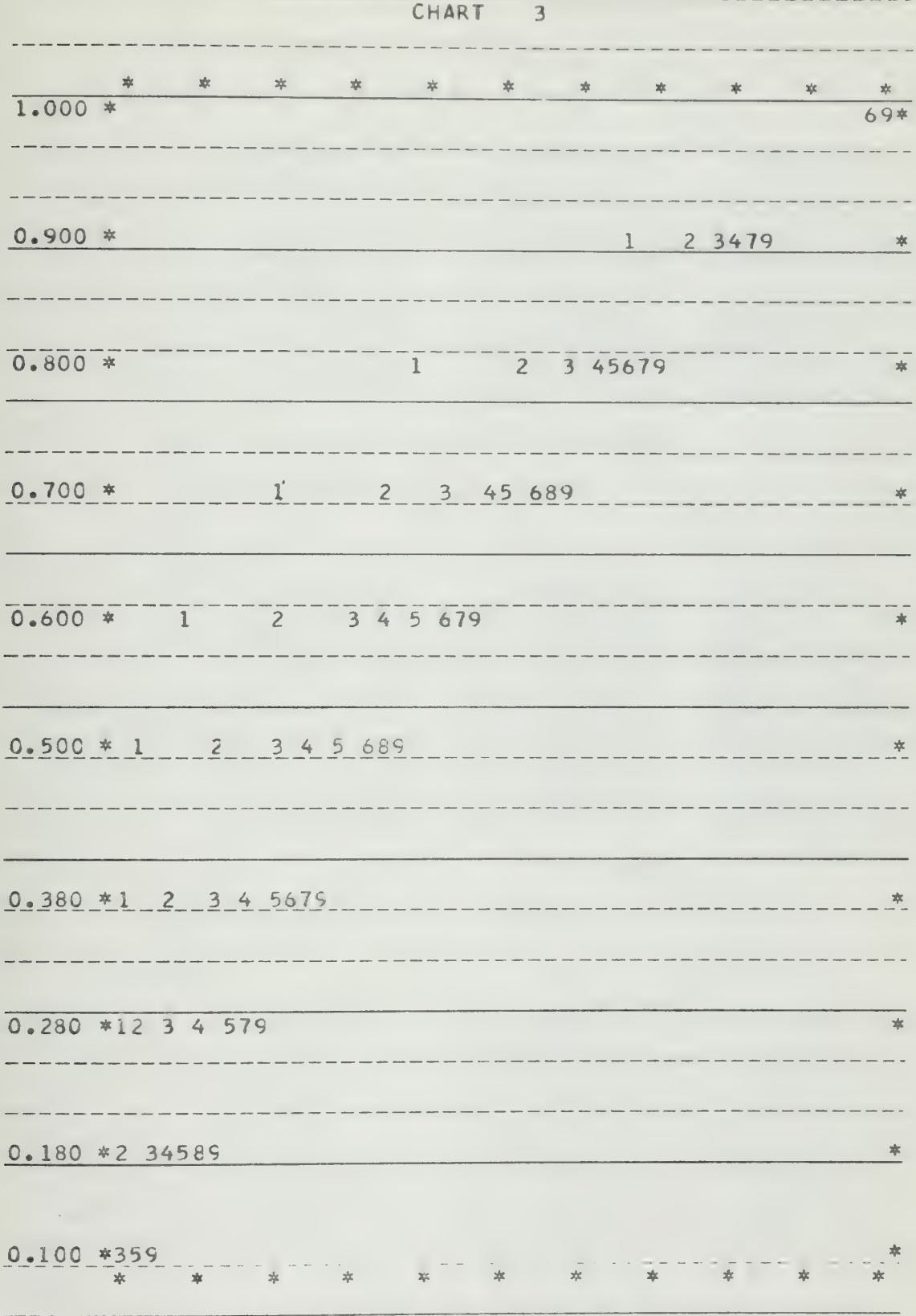
MATRIX 2 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 4

COLUMN 10

ROW	1	0.100000E 01
ROW	2	0.900113E 00
ROW	3	0.802758E 00
ROW	4	0.710389E 00
ROW	5	0.625308E 00
ROW	6	0.549605E 00
ROW	7	0.485104E 00
ROW	8	0.433331E 00
ROW	9	0.395486E 00
ROW	10	0.372433E 00

CHART 3


1.000 * 69*
0.900 * 1 2 3479 *
0.800 * 1 2 3 45679 *
0.700 * 1 2 3 45 689 *
0.600 * 1 2 3 4 5 679 *
0.500 * 1 2 3 4 5 689 *
0.380 *1 2 3 4 5679 *
0.280 *12 3 4 579 *
0.180 *2 34589 *
0.100 *359 *
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.0

MATRIX 3 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 1

	COLUMN	1	2	3
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.900000E 00	0.661296E 00	0.745336E 00
ROW	3	0.800000E 00	0.390233E 00	0.525795E 00
ROW	4	0.700000E 00	0.202861E 00	0.349673E 00
ROW	5	0.600000E 00	0.930687E-01	0.218502E 00
ROW	6	0.500000E 00	0.264024E-01	0.127269E 00
ROW	7	0.400000E 00	0.128419E-01	0.699988E-01
ROW	8	0.300000E 00	0.380260E-02	0.356159E-01
ROW	9	0.200000E 00	0.993013E-03	0.165389E-01
ROW	10	0.100000E 00	0.212133E-03	0.625416E-02

MATRIX 3 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 2

	COLUMN	4	5	6
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.783344E 00	0.806019E 00	0.821203E 00
ROW	3	0.591927E 00	0.632494E 00	0.659998E 00
ROW	4	0.430447E 00	0.482313E 00	0.518177E 00
ROW	5	0.300572E 00	0.356637E 00	0.396426E 00
ROW	6	0.200998E 00	0.254890E 00	0.294283E 00
ROW	7	0.128274E 00	0.174963E 00	0.210224E 00
ROW	8	0.772659E-01	0.113586E 00	0.141865E 00
ROW	9	0.424448E-01	0.667886E-01	0.862302E-01
ROW	10	0.183465E-01	0.303176E-01	0.400413E-01

MATRIX 3 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 3

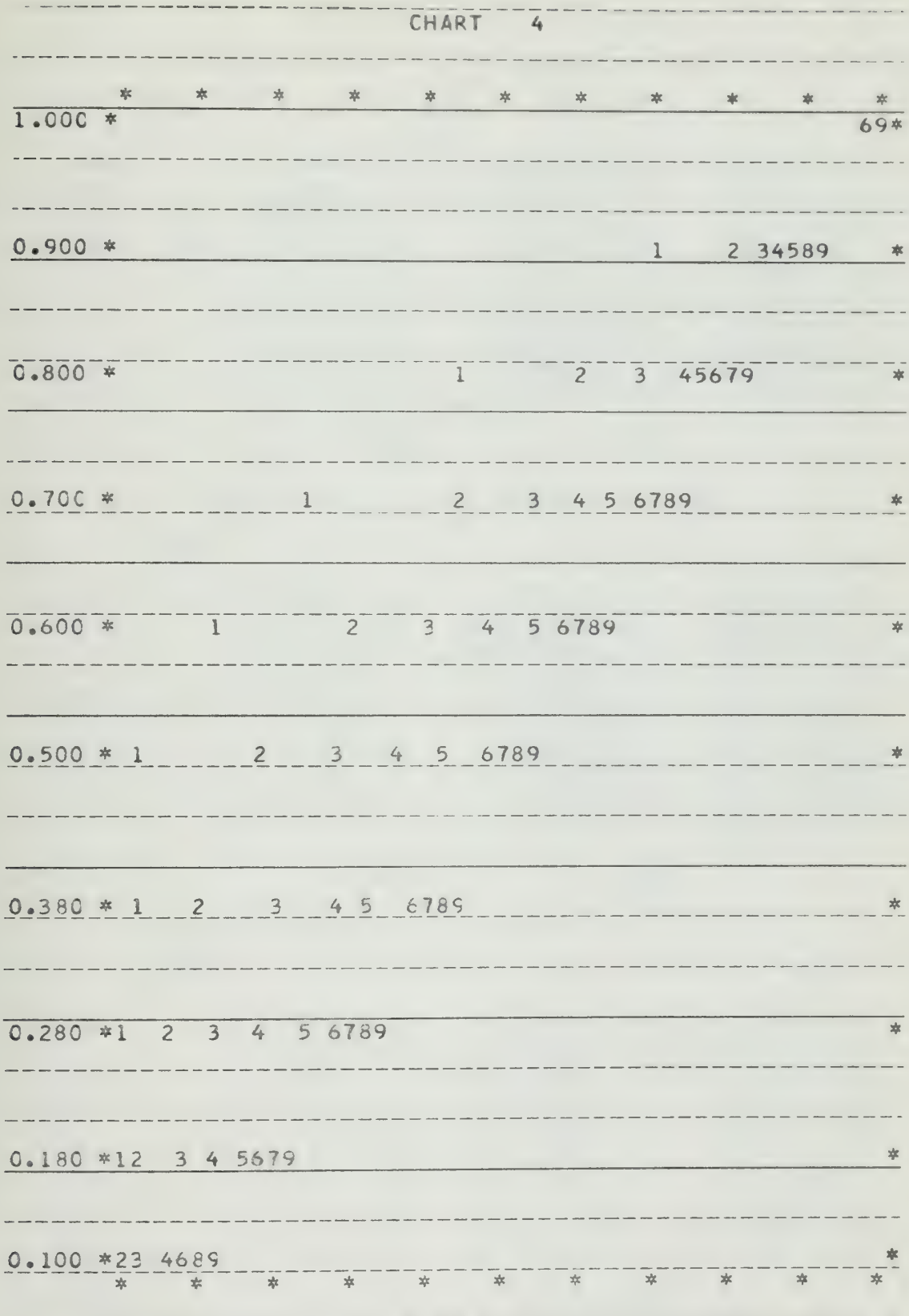
	COLUMN	7	8	9
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.831905E 00	0.839613E 00	0.845214E 00
ROW	3	0.679485E 00	0.693550E 00	0.703780E 00
ROW	4	0.543800E 00	0.562358E 00	0.575874E 00
ROW	5	0.425159E 00	0.446060E 00	0.461308E 00
ROW	6	0.323077E 00	0.344124E 00	0.359509E 00
ROW	7	0.236322E 00	0.255493E 00	0.269533E 00
ROW	8	0.163038E 00	0.178660E 00	0.190122E 00
ROW	9	0.100923E 00	0.111804E 00	0.119797E 00
ROW	10	0.474349E-01	0.529225E-01	0.569578E-01

MATRIX 3 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 4

COLUMN	10
ROW 1	C.100000E 01
ROW 2	0.849298E CC
ROW 3	0.711242E 00
ROW 4	0.585739E 00
ROW 5	0.472445E 00
ROW 6	C.370754E CO
ROW 7	0.279803E 00
ROW 8	0.198512E 00
ROW 9	0.125652E 00
ROW 10	C.599143E-01

CHART 4


1.000 * 69*
0.900 * 1 2 34589 *
0.800 * 1 2 3 45679 *
0.70C * 1 2 3 4 5 6789 *
0.600 * 1 2 3 4 5 6789 *
0.500 * 1 2 3 4 5 6789 *
0.380 * 1 2 3 4 5 6789 *
0.280 *1 2 3 4 5 6789 *
0.180 *12 3 4 5679 *
0.100 *23 4689 *
0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.0

MATRIX 4 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 1

COLUMN		1	2	3
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.900000E 00	0.716376E 00	0.807416E 00
ROW	3	0.800000E 00	0.457947E 00	0.617032E 00
ROW	4	0.700000E 00	0.257891E 00	0.444528E 00
ROW	5	0.600000E 00	0.128171E 00	0.300911E 00
ROW	6	0.500000E 00	0.393896E-01	0.189869E 00
ROW	7	0.400000E 00	0.207545E-01	0.113127E 00
ROW	8	0.300000E 00	0.665832E-02	0.623550E-01
ROW	9	0.200000E 00	0.188375E-02	0.313673E-01
ROW	10	0.100000E 00	0.436425E-03	0.128500E-01

MATRIX 4 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 2

COLUMN		4	5	6
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.848590E 00	0.873154E 00	0.889603E 00
ROW	3	0.694639E 00	0.742246E 00	0.774522E 00
ROW	4	0.547213E 00	0.613148E 00	0.658741E 00
ROW	5	0.413934E 00	0.491145E 00	0.545941E 00
ROW	6	0.299862E 00	0.380262E 00	0.439030E 00
ROW	7	0.207307E 00	0.282761E 00	0.339748E 00
ROW	8	0.135273E 00	0.198860E 00	0.248368E 00
ROW	9	0.804995E-01	0.126669E 00	0.163541E 00
ROW	10	0.376939E-01	0.622888E-01	0.822664E-01

MATRIX 4 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 3

COLUMN		7	8	9
ROW	1	0.100000E 01	0.100000E 01	0.100000E 01
ROW	2	0.901196E 00	0.909546E 00	0.915613E 00
ROW	3	0.797390E 00	0.813896E 00	0.825901E 00
ROW	4	0.691315E 00	0.714908E 00	0.732090E 00
ROW	5	0.585510E 00	0.614294E 00	0.635293E 00
ROW	6	0.481987E 00	0.513387E 00	0.536338E 00
ROW	7	0.381926E 00	0.412908E 00	0.435598E 00
ROW	8	0.285437E 00	0.312787E 00	0.332854E 00
ROW	9	0.191407E 00	0.212042E 00	0.227202E 00
ROW	10	0.974566E-01	0.108731E 00	0.117022E 00

MATRIX 4 10 ROWS 10 COLUMNS

STORAGE MODE 0 GROUP , 4

COLUMN 10

ROW	1	C.100000E 01
ROW	2	0.920038E 0C
ROW	3	0.834659E 00
ROW	4	0.744631E 00
ROW	5	0.650631E 0C
ROW	6	0.553115E 0C
RCW	7	0.452196E 00
ROW	8	0.347543E 00
ROW	9	0.238306E 0C
ROW	10	0.123096E 00

COMPILE TIME= 5.80 SEC,EXECUTION TIME= 5.65 SEC

APPENDIX A5

SUBROUTINES USEFUL FOR COMPUTING LPCM STEADY-STATE SOLUTION

For completeness and for the convenience of the reader, this appendix presents a listing of the Fortran IV statements in the subroutines useful for computing the LPCM steady-state response. As mentioned previously it is expected that there are easier and more efficient methods which could be developed and used to find the steady-state for special cases of the LPCM. These subroutines will solve the general LPCM steady-state with the subroutine AFCT given here. Several of the subroutines here are also used directly in PLPBV, namely EIGEN and GELG.

Four of the subroutines used here are taken, less comment cards, directly from reference (I-3), the Scientific Subroutine Package. These are subroutines LBVP, EIGN, GELG, and LOC. The remaining three subroutines, AFCT, FCT, DFCT, were written specifically for the LPCM. One additional subroutine, OUTP, is required for operation of the subroutine LBVP and must be furnished by the user. All of these subroutines compile under WATFOR in a total time under 20 seconds.

```
C SUBROUTINE LBVP(PRMT,B,C,R,Y,DERY,NDIM,IHLF,AFCT,FCT,DFCT,OUTP,
1AUX,A)
   DIMENSION PRMT(1),B(1),C(1),R(1),Y(1),DERY(1),AUX(20,1),A(1)
   IF(PRMT(3)*(PRMT(2)-PRMT(1)))2,1,3
 1 IHLF=12
   RETURN
 2 IHLF=13
   RETURN
 3 KK=-NDIM
   IB=0
   IC=0
   DO 7 K=1,NDIM
   AUX(15,K)=DERY(K)
   AUX(1,K)=1.
   AUX(17,K)=1.
   KK=KK+NDIM
   DO 4 I=1,NDIM
   II=KK+I
   IF(B(II))5,4,5
 4 CONTINUE
   IB=IB+1
   AUX(1,K)=0.
 5 DO 6 I=1,NDIM
   II=KK+I
   IF(C(II))7,6,7
 6 CONTINUE
   IC=IC+1
   AUX(17,K)=0.
 7 CONTINUE
   IF(IC-IB)8,11,11
 8 H=PRMT(2)
   PRMT(2)=PRMT(1)
   PRMT(1)=H
   PRMT(3)=-PRMT(3)
   DO 9 I=1,NDIM
 9 AUX(17,I)=AUX(1,I)
   II=NDIM*NDIM
   DO 10 I=1,II
   H=B(I)
   B(I)=C(I)
10 C(I)=H
11 X=PRMT(2)
   CALL FCT(X,Y)
   CALL DFCT(X,DERY)
   DO 12 I=1,NDIM
   AUX(18,I)=Y(I)
12 AUX(19,I)=DERY(I)
   K=0
   KK=0
100 K=K+1
   IF(AUX(17,K))108,108,101
101 X=PRMT(2)
   CALL AFCT(X,A)
   SUM=0.
   GL=AUX(18,K)
```

```
      DGL=AUX(19,K)
      II=K
      DO 104 I=1,NDIM
      H=-A(II)
      DERY(I)=H
      AUX(20,I)=R(I)
      Y(I)=0.
      IF(I-K)103,102,103
102   Y(I)=1.
103   DGL=DGL+H*AUX(18,I)
104   II=II+NDIM
      XEND=PRMT(1)
      H=.0625*(XEND-X)
      ISW=0
      GOTO 400
105   IF(IHLF-10)106,106,117
106   DO 107 I=1,NDIM
      KK=KK+1
      H=C(KK)
      R(I)=AUX(20,I)+H*SUM
      II=I
      DO 107 J=1,NDIM
      B(II)=B(II)+H*Y(J)
107   II=II+NDIM
      GOTO 109
108   KK=KK+NDIM
109   IF(K-NDIM)100,110,110
110   X=PRMT(4)
      CALL GELG(R,B,NDIM,1,X,I)
      IF(I)111,112,112
111   IHLF=14
      RETURN
112   PRMT(5)=0.
      IHLF=-I
      X=PRMT(1)
      XEND=PRMT(2)
      H=PRMT(3)
      DO 113 I=1,NDIM
113   Y(I)=R(I)
      ISW=1
114   ISW2=12
      GOTO 200
115   ISW3=-1
      GOTO 300
116   IF(IHLF)400,400,117
117   RETURN
200   CALL AFCT(X,A)
      IF(ISW)201,201,205
201   LL=0
      DO 203 M=1,NDIM
      HS=0.
      DO 202 L=1,NDIM
      LL=LL+1
202   HS=HS-A(LL)*Y(L)
203   DERY(M)=HS
```

```
204 GOTO(502,504,506,407,415,418,608,617,632,634,421,115),ISW2
205 CALL FCT(X,DERY)
    DO 207 M=1,NDIM
    LL=M-NDIM
    HS=0.
    DO 206 L=1,NDIM
    LL=LL+NDIM
206 HS=HS+A(LL)*Y(L)
207 DERY(M)=HS+DERY(M)
    GOTO 204
300 IF(ISW)301,301,305
301 CALL FCT(X,R)
    GU=0.
    DGU=0.
    DO 302 L=1,NDIM
    GU=GU+Y(L)*R(L)
302 DGU=DGU+DERY(L)*R(L)
    CALL DFCT(X,R)
    DO 303 L=1,NDIM
303 DGU=DGU+Y(L)*R(L)
    SUM=SUM+.5*H*((GL+GU)+.1666667*H*(DGL-DGU))
    GL=GU
    DGL=DGU
304 IF(ISW3)116,422,618
305 CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)
    IF(PRMT(5))117,304,117
400 N=1
    XST=X
    IHLF=0
    DO 401 I=1,NDIM
    AUX(16,I)=0.
    AUX(1,I)=Y(I)
401 AUX(8,I)=DERY(I)
    ISW1=1
    GOTO 500
402 X=X+H
    DO 403 I=1,NDIM
403 AUX(2,I)=Y(I)
404 IHLF=IHLF+1
    X=X-H
    DO 405 I=1,NDIM
405 AUX(4,I)=AUX(2,I)
    H=.5*H
    N=1
    ISW1=2
    GOTO 500
406 X=X+H
    ISW2=4
    GOTO 200
407 N=2
    DO 408 I=1,NDIM
    AUX(2,I)=Y(I)
408 AUX(9,I)=DERY(I)
    ISW1=3
    GOTO 500
```

```
409 DO 414 I=1,NDIM
    Z=ABS(Y(I))
    IF(Z-1.)410,411,411
410 Z=1.
411 DELT=.06666667*ABS(Y(I)-AUX(4,I))
    IF(ISW)413,413,412
412 DELT=AUX(15,I)*DELT
413 IF(DELT-Z*PRMT(4))414,414,429
414 CONTINUE
    X=X+H
    ISW2=5
    GOTO 200
415 DO 416 I=1,NDIM
    AUX(3,I)=Y(I)
416 AUX(10,I)=DERY(I)
    N=3
    ISW1=4
    GOTO 500
417 N=1
    X=X+H
    ISW2=6
    GOTO 200
418 X=XST
    DO 419 I=1,NDIM
    AUX(11,I)=DERY(I)
419 Y(I)=AUX(1,I)+H*(.375*AUX(8,I)+.7916667*AUX(9,I)
   1-.2083333*AUX(10,I)+.04166667*DERY(I))
420 X=X+H
    N=N+1
    ISW2=11
    GOTO 200
421 ISW3=0
    GOTO 300
422 IF(N-4)423,600,600
423 DO 424 I=1,NDIM
    AUX(N,I)=Y(I)
424 AUX(N+7,I)=DERY(I)
    IF(N-3)425,427,600
425 DO 426 I=1,NDIM
    DELT=AUX(9,I)+AUX(9,I)
    DELT=DELT+DELT
426 Y(I)=AUX(1,I)+.3333333*H*(AUX(8,I)+DELT+AUX(10,I))
    GOTO 420
427 DO 428 I=1,NDIM
    DELT=AUX(9,I)+AUX(10,I)
    DELT=DELT+DELT+DELT
428 Y(I)=AUX(1,I)+.375*H*(AUX(8,I)+DELT+AUX(11,I))
    GOTO 420
429 IF(IHLF-10)404,430,430
430 IHLF=11
    X=X+H
    IF(ISW)105,105,114
500 Z=X
    DO 501 I=1,NDIM
    X=H*AUX(N+7,I)
```

```
      AUX(5,I)=X
  501 Y(I)=AUX(N,I)+.4*X
      X=Z+.4*H
      ISW2=1
      GOTO 200
  502 DO 503 I=1,NDIM
      X=H*DERY(I)
      AUX(6,I)=X
  503 Y(I)=AUX(N,I)+.2969776*AUX(5,I)+.1587596*X
      X=Z+.4557372*H
      ISW2=2
      GOTO 200
  504 DO 505 I=1,NDIM
      X=H*DERY(I)
      AUX(7,I)=X
  505 Y(I)=AUX(N,I)+.2181004*AUX(5,I)-3.050965*AUX(6,I)+3.832865*X
      X=Z+H
      ISW2=3
      GOTO 200
  506 DO 507 I=1,NDIM
  507 Y(I)=AUX(N,I)+.1747603*AUX(5,I)-.5514807*AUX(6,I)
     1+1.205536*AUX(7,I)+.1711848*H*DERY(I)
      X=Z
      GOTO(402,406,409,417),ISW1
  600 ISTEP=3
  601 IF(N-8)604,602,604
  602 DO 603 N=2,7
      DO 603 I=1,NDIM
      AUX(N-1,I)=AUX(N,I)
  603 AUX(N+6,I)=AUX(N+7,I)
      N=7
  604 N=N+1
      DO 605 I=1,NDIM
      AUX(N-1,I)=Y(I)
  605 AUX(N+6,I)=DERY(I)
      X=X+H
  606 ISTEP=ISTEP+1
      DO 607 I=1,NDIM
     0DELT=AUX(N-4,I)+1.333333*H*(AUX(N+6,I)+AUX(N+6,I)-AUX(N+5,I)+
     1AUX(N+4,I)+AUX(N+4,I))
      Y(I)=DELT-.9256198*AUX(16,I)
  607 AUX(16,I)=DELT
      ISW2=7
      GOTO 200
  608 DO 609 I=1,NDIM
     0DELT=.125*(9.*AUX(N-1,I)-AUX(N-3,I)+3.*H*(DERY(I)+AUX(N+6,I)+
     1AUX(N+6,I)-AUX(N+5,I)))
      AUX(16,I)=AUX(16,I)-DELT
  609 Y(I)=DELT+.0743801 7*AUX(16,I)
      DELT=0.
      DO 616 I=1,NDIM
      Z=ABS(Y(I))
      IF(Z-1.)610,611,611
  610 Z=1.
  611 Z=ABS(AUX(16,I))/Z
```

```
      IF(ISW)613,613,612
  612 Z=AUX(15,I)*Z
  613 IF(Z-PRMT(4))614,614,628
  614 IF(DELT-Z)615,616,616
  615 DELT=Z
  616 CONTINUE
      ISW2=8
      GOTO 200
  617 ISW3=1
      GOTO 300
  618 IF(H*(X-XEND))619,621,621
  619 IF(ABS(X-XEND)-.1*ABS(H))621,620,620
  620 IF(DELT-.02*PRMT(4))622,622,601
  621 IF(ISW)105,105,117
  622 IF(IHLF)601,601,623
  623 IF(N-7)601,624,624
  624 IF(ISTEP-4)601,625,625
  625 IMOD=ISTEP/2
      IF(ISTEP-IMOD-IMOD)601,626,601
  626 H=H+H
      IHLF=IHLF-1
      ISTEP=0
      DO 627 I=1,NDIM
      AUX(N-1,I)=AUX(N-2,I)
      AUX(N-2,I)=AUX(N-4,I)
      AUX(N-3,I)=AUX(N-6,I)
      AUX(N+6,I)=AUX(N+5,I)
      AUX(N+5,I)=AUX(N+3,I)
      AUX(N+4,I)=AUX(N+1,I)
      DELT=AUX(N+6,I)+AUX(N+5,I)
      DELT=DELT+DELT+DELT
 6270AUX(16,I)=8.962963*(Y(I)-AUX(N-3,I))-3.361111*H*(DERY(I)+DELT
     1+AUX(N+4,I))
      GOTO 601
  628 IHLF=IHLF+1
      IF(IHLF-10)630,630,629
  629 IF(ISW)105,105,114
  630 H=.5*H
      ISTEP=0
      DO 631 I=1,NDIM
     0Y(I)=.00390625*(80.*AUX(N-1,I)+135.*AUX(N-2,I)+40.*AUX(N-3,I)+
     1AUX(N-4,I))-.1171875*(AUX(N+6,I)-6.*AUX(N+5,I)-AUX(N+4,I))*H
     0AUX(N-4,I)=.00390625*(12.*AUX(N-1,I)+135.*AUX(N-2,I)+
     1108.*AUX(N-3,I)+AUX(N-4,I))-.0234375*(AUX(N+6,I)+18.*AUX(N+5,I)-
     29.*AUX(N+4,I))*H
      AUX(N-3,I)=AUX(N-2,I)
  631 AUX(N+4,I)=AUX(N+5,I)
      DELT=X-H
      X=DELT-(H+H)
      ISW2=9
      GOTO 200
  632 DO 633 I=1,NDIM
      AUX(N-2,I)=Y(I)
      AUX(N+5,I)=DERY(I)
  633 Y(I)=AUX(N-4,I)
```

```
      X=X-(H+H)
      ISW2=10
      GOTO 200
34    X=DELT
      DO 635 I=1,NDIM
      DELT=AUX(N+5,I)+AUX(N+4,I)
      DELT=DELT+DELT+DELT
     CAUX(16,I)=8.962963*(AUX(N-1,I)-Y(I))-3.361111*H*(AUX(N+6,I)+DELT
     1+DERY(I))
35    AUX(N+3,I)=DERY(I)
      GOTO 606
      END
```

```
      SUBROUTINE GELG(R,A,M,N,EPS,IER)
      DIMENSION A(1),R(1)
      IF(M)23,23,1
    1 IER=0
      PIV=0.
      MM=M*M
      NM=N*M
      DO 3 L=1,MM
      TB=ABS(A(L))
      IF(TB-PIV)3,3,2
    2 PIV=TB
      I=L
    3 CONTINUE
      TOL=EPS*PIV
      LST=1
      DO 17 K=1,M
      IF(PIV)23,23,4
    4 IF(IER)7,5,7
    5 IF(PIV-TOL)6,6,7
    6 IER=K-1
    7 PIVI=1./A(I)
      J=(I-1)/M
      I=I-J*M-K
      J=J+1-K
      DO 8 L=K,NM,M
      LL=L+I
      TB=PIVI*R(LL)
      R(LL)=R(L)
    8 R(L)=TB
      IF(K-M)9,18,18
    9 LEND=LST+M-K
      IF(J)12,12,10
   10 II=J*M
      DO 11 L=LST,LEND
      TB=A(L)
      LL=L+II
      A(L)=A(LL)
   11 A(LL)=TB
   12 DO 13 L=LST,MM,M
      LL=L+I
      TB=PIVI*A(LL)
      A(LL)=A(L)
   13 A(L)=TB
      A(LST)=J
      PIV=0.
      LST=LST+1
      J=0
      DO 16 II=LST,LEND
      PIVI=-A(II)
      IST=II+M
      J=J+1
      DO 15 L=IST,MM,M
      LL=L-J
      A(L)=A(L)+PIVI*A(LL)
      TB=ABS(A(L))
```

```
      IF(TB-PIV)15,15,14
   14 PIV=TB
      I=L
   15 CONTINUE
      DO 16 L=K,NM,M
      LL=L+J
   16 R(LL)=R(LL)+PIVI*R(L)
   17 LST=LST+M
   18 IF(M-1)23,22,19
   19 IST=MM+M
      LST=M+1
      DO 21 I=2,M
      II=LST-I
      IST=IST-LST
      L=IST-M
      L=A(L)+.5
      DO 21 J=II,NM,M
      TB=R(J)
      LL=J
      DO 20 K=IST,MM,M
      LL=LL+1
   20 TB=TB-A(K)*R(LL)
      K=J+L
      R(J)=R(K)
   21 R(K)=TB
   22 RETURN
   23 IER=-1
      RETURN
      END
```

```
      SUBROUTINE AFCT(X,A)
C     THIS SUBROUTINE IS A PORTION OF PLPBV
C
C     THESE DIMENSIONS MUST BE CHANGED IF THE INPUT
C     POLYNOMIAL DIMENSIONS OF PLPBV ARE CHANGED.
      DIMENSION P(3),Q(3)
C
C     MATRIX A MUST BE IN VECTOR FORM
C
      DIMENSION A(1)
C
C        P,Q, AND N ARE POLYNOMIAL COEFFICIENTS AND MUST BE
C        MAIN PROGRAM AND PLACED IN COMMON AREA S .
C
      COMMON /S/P,Q,N
C        EPSILON IS ZERO VALUE FOR THIS SUBROUTINE
      EPS=1.0E-07
      P1=P(1)
      P3=Q(1)
      P4=0.0
      IF(N-1)10,11,12
   11 P1=P1+P(2)*X
      P4=Q(2)
      GO TO 10
   12 P1=P1+P(2)*X
      P3=P3+2.0*P(2)+Q(2)*X
      P4=Q(2)
      XIMM=1.0
      DO 20 I=2,N
      XIM=XIMM*X
      XI=XIM*X
      RI=FLOAT(I)
      P1=P1+P(I+1)*XI
      P3=P3+2.0*RI*P(I+1)*XIM+Q(I+1)*XI
      P4=P4+RI*((RI-1.0)*P(I+1)*XIMM+Q(I+1)*XIM)
      XIMM=XIMM*X
   20 CONTINUE
   10 IF(ABS(P1)-EPS)13,13,14
   13 A(2)=0.0
      A(3)=0.0
      A(4)=0.0
      IF(ABS(P3)-EPS)15,15,16
   15 A(1)=0.0
      RETURN
   16 A(1)=-P4/P3
      RETURN
   14 A(1)=0.0
      A(2)=-P4/P1
      A(3)=1.0
      A(4)=-P3/P1
      RETURN
      END
```

```
      SUBROUTINE FCT(X,F)
C     THIS SUBROUTINE IS A PORTION OF PLPBV
      DIMENSION F(2)
      F(1)=0.0
      F(2)=0.0
      RETURN
      END
```

```
      SUBROUTINE DFCT(X,DF)
C     THIS SUBROUTINE IS A PORTION OF PLPBV
      DIMENSION DF(2)
      DF(1)=0.0
      DF(2)=0.0
      RETURN
      END
```

```
      SUBROUTINE LOC(I,J,IR,N,M,MS)
      IX=I
      JX=J
      IF(MS-1) 10,20,30
   10 IRX=N*(JX-1)+IX
      GO TO 36
   20 IF(IX-JX) 22,24,24
   22 IRX=IX+(JX*JX-JX)/2
      GO TO 36
   24 IRX=JX+(IX*IX-IX)/2
      GO TO 36
   30 IRX=0
      IF(IX-JX) 36,32,36
   32 IRX=IX
   36 IR=IRX
      RETURN
      END
```

```
      SUBROUTINE FCT(X,F)
C     THIS SUBROUTINE IS A PORTION OF PLPBV
      DIMENSION F(2)
      F(1)=0.0
      F(2)=0.0
      RETURN
      END
```

```
      SUBROUTINE DFCT(X,DF)
C     THIS SUBROUTINE IS A PORTION OF PLPBV
      DIMENSION DF(2)
      DF(1)=0.0
      DF(2)=0.0
      RETURN
      END
```

```
      SUBROUTINE LOC(I,J,IR,N,M,MS)
      IX=I
      JX=J
      IF(MS-1) 10,20,30
   10 IRX=N*(JX-1)+IX
      GO TO 36
   20 IF(IX-JX) 22,24,24
   22 IRX=IX+(JX*JX-JX)/2
      GO TO 36
   24 IRX=JX+(IX*IX-IX)/2
      GO TO 36
   30 IRX=0
      IF(IX-JX) 36,32,36
   32 IRX=IX
   36 IR=IRX
      RETURN
      END
```

```
      SUBROUTINE EIGEN(A,R,N,MV)
      DIMENSION A(1),R(1)
    5 RANGE=1.0E-6
      IF(MV-1) 10,25,10
   10 IQ=-N
      DO 20 J=1,N
      IQ=IQ+N
      DO 20 I=1,N
      IJ=IQ+I
      R(IJ)=0.0
      IF(I-J) 20,15,20
   15 R(IJ)=1.0
   20 CONTINUE
   25 ANORM=0.0
      DO 35 I=1,N
      DO 35 J=I,N
      IF(I-J) 30,35,30
   30 IA=I+(J*J-J)/2
      ANORM=ANORM+A(IA)*A(IA)
   35 CONTINUE
      IF(ANORM) 165,165,40
   40 ANORM=1.414*SQRT(ANORM)
      ANRMX=ANORM*RANGE/FLOAT(N)
      IND=0
      THR=ANORM
   45 THR=THR/FLOAT(N)
   50 L=1
   55 M=L+1
   60 MQ=(M*M-M)/2
      LQ=(L*L-L)/2
      LM=L+MQ
   62 IF( ABS(A(LM))-THR) 130,65,65
   65 IND=1
      LL=L+LQ
      MM=M+MQ
      X=0.5*(A(LL)-A(MM))
   68 Y=-A(LM)/ SQRT(A(LM)*A(LM)+X*X)
      IF(X) 70,75,75
   70 Y=-Y
   75 SINX=Y/ SQRT(2.0*(1.0+( SQRT(1.0-Y*Y))))
      SINX2=SINX*SINX
   78 COSX= SQRT(1.0-SINX2)
      COSX2=COSX*COSX
      SINCS =SINX*COSX
      ILQ=N*(L-1)
      IMQ=N*(M-1)
      DO 125 I=1,N
      IQ=(I*I-I)/2
      IF(I-L) 80,115,80
   80 IF(I-M) 85,115,90
   85 IM=I+MQ
      GO TO 95
   90 IM=M+IQ
   95 IF(I-L) 100,105,105
  100 IL=I+LQ
```

```
      GO TO 110
  105 IL=L+IQ
  110 X=A(IL)*COSX-A(IM)*SINX
      A(IM)=A(IL)*SINX+A(IM)*COSX
      A(IL)=X
  115 IF(MV-1) 120,125,120
  120 ILR=ILQ+I
      IMR=IMQ+I
      X=R(ILR)*COSX-R(IMR)*SINX
      R(IMR)=R(ILR)*SINX+R(IMR)*COSX
      R(ILR)=X
  125 CONTINUE
      X=2.0*A(LM)*SINCS
      Y=A(LL)*COSX2+A(MM)*SINX2-X
      X=A(LL)*SINX2+A(MM)*COSX2+X
      A(LM)=(A(LL)-A(MM))*SINCS+A(LM)*(COSX2-SINX2)
      A(LL)=Y
      A(MM)=X
  130 IF(M-N) 135,140,135
  135 M=M+1
      GO TO 60
  140 IF(L-(N-1)) 145,150,145
  145 L=L+1
      GO TO 55
  150 IF(IND-1) 160,155,160
  155 IND=0
      GO TO 50
  160 IF(THR-ANRMX) 165,165,45
  165 IQ=-N
      DO 185 I=1,N
      IQ=IQ+N
      LL=I+(I*I-I)/2
      JQ=N*(I-2)
      DO 185 J=I,N
      JQ=JQ+N
      MM=J+(J*J-J)/2
      IF(A(LL)-A(MM)) 170,185,185
  170 X=A(LL)
      A(LL)=A(MM)
      A(MM)=X
      IF(MV-1) 175,185,175
  175 DO 180 K=1,N
      ILR=IQ+K
      IMR=JQ+K
      X=R(ILR)
      R(ILR)=R(IMR)
  180 R(IMR)=X
  185 CONTINUE
      RETURN
      END
```

APPENDIX A6

SUBROUTINE PLPBV

This appendix presents a complete listing of a suggested format and some of the computation statements necessary to solve the PLPBV model which is a special case of the LPCM. As stated in the subroutine description, the program presented here is incomplete and represents at best a format for further use developing the complete solution to the LPCM utilizing the integral equation methods of this thesis.

One important result of the use of this subroutine is that the total computation time necessary for solution is very short. Subroutine PLPBV, the MAIN program calling it, and all of the subroutines used compiled under WATFOR in 12 seconds and executed completely in 15 seconds. More elaborate programs would undoubtedly require more than 15 seconds computation time, but the fact that a problem as general as PLPBV can be solved in a time this short is very encouraging for more general versions of the LPCM. A flowchart of PLPBV is presented in Chapter L2.

For completeness, the MAIN program used to call PLPBV as a test is presented at the end of this appendix. In general, this main program would employ the approximations and combinations of upper and lower solutions for a complete distillation column modeling using PLPBV to solve the upper and lower versions of the LPCM.

```
      SUBROUTINE PLPBV(PRMT,P,Q,N,BC,F,US,UT,U)
C
C *** NOTE ***************************************************
C     THIS PROGRAM IS INCOMPLETE IN SEVERAL ASPECTS AND
C     REQUIRES EXTENSIVE WORK TO BE USEFUL IN GENERAL
C     PURPOSE COMPUTATION.
C     SUBROUTINE PLPBV IS PRESENTED HERE AS A FORMAT FOR
C     AND EXAMPLE OF THE STEPS NECESSARY TO APPLY THE
C     INTEGRAL EQUATION TECHNIQUE OF THIS THESIS.
C *** NOTE ***************************************************
C
C
C     ***********************************************************
C
C          SUBROUTINE PLPBV(PRMT,P,Q,N,BC,F,US,UT,U)
C
C          PURPOSE
C             TO SOLVE A LINEAR,SECCND CRDER,PARABOLIC,
C             PARTIAL DIFFERENTIAL EQUATION WITH BOUNDARY
C             CONDITIONS AND POLYNOMIAL COEFFICIENTS,
C             D/DXX(P(X)U(X,T))+D/DX(Q(X)U(X,T))=D/DT(U(X,T))
C             WHERE P AND Q ARE POLYNOMIALS IN X, IN RESPONSE
C             TO STEP INPUTS,WHERE F IS STEADY STATE AT T=TL.
C
C          USAGE
C             CALL PLPBV(PRMT,P,Q,N,BC,F,US,UT,U)
C
C          DESCRIPTION OF PARAMETERS
C             F       -INPUT STEADY-STATE DISTRIBUTION AT TL
C             BC      -INPUT BOUNDARY CONDITIONS OF THE FORM
C                        BC(7)U+BC(9)UX=BC(1) AT X=XU
C                        BC(4)U+BC(6)UX=BC(2) AT X=XL
C                        BC MUST BE AT LEAST OF DIMENSION 10
C                        PLPBV SETS BC(3,5,8,10)=0 FOR LBVP USE
C             PRMT    - INPUT VECTOR WHICH SPECIFIES THE PARA-
C                        METERS OF THE X AND T INTERVALS AND OF
C                        THE ACCURACY FOR SUBROUTINES USED BY
C                        PLPBV, MUST BE AT LEAST DIMENSION 10
C             PRMT(1)- LOWER BOUND XL OF THE X VARIABLE
C             PRMT(1)- UPPER BOUND XU OF THE X VARIABLE
C             PRMT(3)- SPATIAL INCREMENT OF THE X VARIABLE
C             PRMT(4)- UPPER ERROR BOUND FOR X
C             PRMT(5)- TERMINATION PARAMETER FOR X
C             PRMT(6)- LOWER BOUND TL OF THE T VARIABLE
C             PRMT(7)- UPPER BOUND TU OF THE T VARIABLE
C             PRMT(8)- TIME INCREMENT OF THE T VARIABLE
C             PRMT(9)- ERROR WEIGHT LTE 1.0 FOR LBVP USE
C             PRMT(10) ERROR WEIGHT LTE 1.0 FOR LBVP USE
C                        BOTH ERROR WEIGHTS ARE USUALLY 1.0
C             P       - INPUT VECTOR SPECIFYING THE
C                        COEFFICIENTS OF THE FIRST
C                        POLYNOMIAL OF DEGREE N
C             Q       - INPUT VECTOR SPECIFYING THE
C                        COEFFICIENTS OF THE SECOND
C                        POLYNOMIAL OF DEGREE N
```

```
C             N       - INPUT SPECIFYING THE MAXIMUM
C                       DEGREE OF P AND Q
C                       THE COEFFICIENTS MUST BE IN THE
C                       ORDER OF LOW TO HIGH INDEX
C                       CORRESPONDING TO LOW TO HIGH
C                       DEGREE IN EACH POLYNOMIAL
C                       BOTH P AND Q MUST BE AT LEAST OF
C                       DIMENSION N WITH THE REMAINING
C                       COEFFICIENTS IN EITHER P OR Q SET=0
C             US      - OUTPUT STEADY-STATE SPATIAL
C                       DISTRIBUTION VECTOR
C             UT      - OUTPUT TRANSIENT RESPONSE
C             U       - OUTPUT U=US+UT OVERALL SOLUTION TO THE
C                       TWO POINT BOUNDARY VALUE, STEP INITIAL
C                       VALUE PROBLEM.
C
C          REMARKS
C             (1) STEADY-STATE PORTION WRITTEN FOR MAX N=3,
C                 THIS CAN BE EASILY CHANGED BY USING
C                 DIFFERENT DIMENSION STATEMENTS ON P AND Q
C             (2) TRANSIENT PORTION WRITTEN FOR P(1),Q(1),
C                 AND Q(2), CHANGING THIS REQUIRES ANALYTICAL
C                 APPLICATION OF THE INTEGRAL EQUATION
C                 TECHNIQUE PRESENTED IN THIS THESIS.
C             (3) THIS SUBROUTINE HAS BEEN INITIALLY WRITTEN
C                 TO EVALUATE AT TEN POINTS IN X AND AT NINE
C                 POINTS IN T. THIS COULD BE CHANGED TO A
C                 MORE GENERAL METHOD IF DESIRED.
C             (4) THERE ARE SEVERAL ERROR OUTPUTS IN PLPBV.
C             (5) SUBROUTINE PLPBV HAS NOT BEEN OPTIMIZED.
C             (6) SUBROUTINE PLPBV HAS BEEN WRITTEN MAINLY TO
C                 DEMONSTRATE THE STEPS NECESSARY TO APPLY
C                 THE INTEGRAL EQUATION SOLUTION OF THIS THESIS.
C             (7) IT IS EXPECTED THAT SEVERAL 'BUGS' REMAIN
C                 IN SUBROUTINE PLPBV AS WRITTEN HERE.
C             (8) AS THE AFCT OF APPENDIX A5 IS NOW WRITTEN,
C                 A STATEMENT, COMMON /S/P,Q,N  ,IS REQUIRED
C                 IN THE MAIN PROGRAM. THIS COULD BE CHANGED
C                 BY INCREASING THE PARAMETER DIMENSIONS IN
C                 SUBROUTINE AFCT.
C
C          SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED
C             SUBROUTINE PLPBV REQUIRES IBM/SSP SUBROUTINES-
C               LBVP, GELG, EIGEN, AND LOC
C             AND USER FURNISHED SUBROUTINES-
C               AFCT, DFCT, FCT, AND OUTP FOR USE IN LBVP
C
C     ***************************************************
C
      DIMENSION PRMT(1),P(1),Q(1),BC(1),F(1),US(1),UT(1),U(1)
      DIMENSION D(4),AK(100),UZ(10),XI(100),XJ(100)
      DIMENSION AKS(55),TH(10),EIG(100),TLAM(10),WI(100)
C
C     INPUT AND PARAMETER SETUP SECTION
      NDIM=2
```

```
      NV=10
      NT=9
      CN=10.0
      CT=8.0
      EPS=1.0E-05
      AA=PRMT(1)
      BB=PRMT(2)
      TL=PRMT(6)
      THH=PRMT(7)
      IF(ABS(P(1))-EPS)33,33,34
   33 WRITE(6,35)P(1)
   35 FORMAT(1X,'P(1) INVALID, P(1)=  ',E15.7,//)
      RETURN
   34 SPZ=SQRT(P(1))
      SSPZ=SQRT(SPZ)
C
C     STEADY STATE SECTION, USES SUBROUTINE LBVP
C     STEADY-STATE VALUES RETURNED THROUGH XPAR
      DIMENSION Y(2),DERY(2),AV(4),AUX(20,2)
      DIMENSION R(2),B(4),C(4),TPAR(15),XPAR(15)
      EXTERNAL FCT,DFCT,AFCT,OUTP
      DO 55 I=1,5
      XPAR(I)=PRMT(I)
      TPAR(I)=PRMT(I+5)
   55 CONTINUE
      R(1)=BC(1)
      R(2)=BC(2)
      BC(3)=0.0
      BC(5)=0.0
      BC(8)=0.0
      BC(10)=0.0
      DO 56 I=1,4
      B(I)=BC(I+2)
      C(I)=BC(I+6)
   56 CONTINUE
      DERY(1)=PRMT(9)
      DERY(2)=PRMT(10)
      CALL LBVP(XPAR,B,C,R,Y,DERY,NDIM,IHLF,AFCT,FCT,DFCT,
     1OUTP,AUX,AV)
C
C     TESTS APPLIED UPON RETURN FROM LBVP
      IF(IHLF-13)39,40,41
   41 WRITE(6,42)
   42 FORMAT(1X,'LBVP HAS IHLF=14, NO SOLUTION ',//)
      RETURN
   39 IF(IHLF-11)44,45,40
   45 WRITE(6,46)
   46 FORMAT(1X,'LBVP HAS IHLF GT 10, NO SOLUTION',//)
      RETURN
   40 WRITE(6,43)
   43 FORMAT(1X,'LBVP HAS IHLF=13 OR 12, PARAMETER ERROR',//)
      RETURN
   44 WRITE(6,47)IHLF
   47 FORMAT(1X,'LBVP RETURN SATISFACTORY, IHLF=  ',I3,//)
C
```

```
C
C     TRANSIENT SECTION, USES SUBROUTINES EIGEN AND GELG
C
C     TRANSFORMING BOUNDARY CONDITIONS
      D(1)=BC(7)-(BC(9)*(Q(1)+Q(2)*PRMT(2)))/(2.0*P(1))
      D(2)=BC(4)-(BC(6)*(Q(1)+Q(2)*PRMT(1)))/(2.0*P(1))
      D(3)=BC(9)/SPZ
      D(4)=BC(6)/SPZ
      DTEST=D(1)*D(4)-D(2)*D(3)
      CONE=D(1)*D(2)-DTEST
      IF(ABS(CONE)-EPS)31,31,30
   31 WRITE(6,32)CONE
   32 FORMAT(1X,'C1 IS ',E15.7,'SETTING C1 TO 1.E-05 ',//)
      CONE=EPS
C     SET UP INTERVAL FOR KERNEL EVALUATION
   30 DELTX=(PRMT(2)-PRMT(1))/CN
      CC=DELTX*CN/P(1)
C
C     PROGRAM RUNS FOR 10 DELTX AND 10 DELTZ
C     FOR GREATER ACCURACY MORE INCREMENTS COULD BE USED
      DELTZ=CC/CN
C
C     BEGIN KERNEL EVALUATIONS
      EMZ=1.5*Q(2)+0.25*Q(1)*Q(1)/P(1)
C
C     SEVERAL ALTERNATIVE KERNEL EVALUATION ROUTINES
C     MUST BE DESIGNED AND PLACED IN THIS SECTION FOR
C     CASES SUCH AS **
C          (1) M(0)=0
C          (2) M(Z)=M(0)
C     AND OTHERS.
C     THESE ROUTINES MUST USE EQUATIONS A1.23 AND A1.24
C     OF THIS THESIS.
C
C     TEST M(0)
      IF(ABS(EMZ)-EPS)50,50,51
   50 WRITE(6,52)EMZ
   52 FORMAT(1X,'M(0)=0 , INVALID FOR PLPBV,  M(0)=',E15.7,//)
      RETURN
   51 DK=D(1)+D(3)
      FP=4.0*P(1)
      LK=0
      LS=0
      DO 49 JK=1,NV
      DO 48 IK=1,NV
C     COMPUTE K4(Z,S)
      LK=LK+1
      Z=IK*DELTZ
      S=JK*DELTZ
      XS=SPZ*S+AA
      CMS=CC-S
      DMDZ=(D(4)-D(2)*Z)/CONE
      XCMS=SPZ*CMS+AA
      EMS=EMZ+(2.0*Q(1)*Q(2)*XS+Q(2)*Q(2)*XS*XS)/FP
      XQ=Q(2)*XCMS
```

```
      EMCMS=EMZ+(2.0*Q(1)*XQ+XQ*XQ)/FP
      KF=DMDZ*(D(1)*EMCMS+D(3)*EMS-DK*EMZ)/EMZ
      IF(IK-JK)54,54,53
   54 AK(LK)=KF
      LS=LS+1
      AKS(LS)=KF                        Note:  obvious error
      GO TO 48                            KF should be RKF, real.
   53 ZMS=Z-S
      XZMS=SPZ*ZMS+AA
      XQZ=Q(2)*XZMS
      AK(LK)=((2.0*Q(1)*XQZ+XQZ*XQZ)/(EMZ*FP))+KF
   48 CONTINUE
   49 CONTINUE
C
C     COMPUTE EIGENVALUES AND EIGENVECTORS OF AKS
      MV=0
      CALL EIGEN(AKS,EIG,NV,MV)
C
C     TAKE EIGENVALUES TH(I) FROM DIAGONAL OF AKS(I)
      EPTH=1.0E-10
      IS=1
      DO 60 I=1,NV
      TH(I)=AKS(IS)
      IS=IS+(I+1)
      IF(TH(I)-EPTH)57,57,58
   58 TLAM(I)=1.0/(TH(I)*DELTZ)
      GO TO 60
   57 WRITE(6,74)TH(I),I
   74 FORMAT(1X,'THETA(I) INVALID, TH(I)=',E15.7,'   I=',I3)
      WRITE(6,59)
   59 FORMAT(1X,'SETTING TH(I)=EPTH',/)
      TLAM(I)=EPTH
   60 CONTINUE
C
C     THIS PROGRAM HAS BEEN SET UP SO THAT DELTX AND DELTZ
C     CORRESPOND. THIS MAKES WI(ZI)=WI(XI). IF THIS WERE
C     NOT DESIRED, THEN A SECTION UTILIZING EQUATION A3.10
C     WOULD HAVE TO BE EMPLOYED.
C
C     COMPUTE WI(X) FROM WI(Z), THETA(I)=TH(I),WI(Z)=EIG(Z)
      IJ=0
      DO 63 I=1,NV
      DO 64 J=1,NV
      IJ=IJ+1
      WI(IJ)=EIG(IJ)
   64 CONTINUE
   63 CONTINUE
C
C     TRANSFORM WI(X) TO XI(X)
      X=DELTX+AA
      DO 61 J=1,NV
      XMA=X-AA
      XPA=X+AA
      XFUN=(XMA*Q(1))/(2.0*P(1))+(XMA*XPA*Q(2))/FP
      EXX=EXP(-XFUN)*SSPZ
```

```
      X=X+DELTX
      DO 62 I=1,NV
      JI=J+NV*(I-1)
      XI(JI)=EXX*WI(JI)
   62 CONTINUE
   61 CONTINUE
C
C     BEGIN EIGENFUNCTION EXPANSION TO MEET INITIAL CONDITION.
      DELTT=(THH-TL)/CT
      T=TL
C
C     FORM STEADY-STATE VECTOR
      DO 65 I=1,NV
      UZ(I)=F(I)-US(I)
   65 CONTINUE
C
C     FORM EXPANSION MATRIX,XJ(X), AT T=TL
      IJ=0
      DO 66 I=1,NV
      EXT=EXP(-TLAM(I)*T)
      DO 67 J=1,NV
      IJ=IJ+1
      XJ(IJ)=XI(IJ)*EXT
   67 CONTINUE
   66 CONTINUE
C
C     SOLVE SIMULTANEOUS EQUATIONS FOR EIGENFUNCTION
C     CONSTANTS USING SUBROUTINE GELG
      NG=1
      CALL GELG(UZ,XJ,NV,NG,EPS,IER)
C
C     TEST IER UPON RETURN FROM GELG
      IF(IER)36,37,38
   36 WRITE(6,68)
   68 FORMAT(1X,'NO RESULT,PIVOT ELEMENT=0 IN GELG ',/)
      RETURN
   38 WRITE(6,69)
   69 FORMAT(1X,'POSSIBLE LOSS OF SIGNIFICANCE IN GELG',/)
C
C     THIS SECTION SETS UP U(X,T) IN A FORM ACCEPTIBLE
C     FOR PLOTTING BY SUBROUTINE PLOT OF APPENDIX A4.
C     THE FIRST COLUMN OF U(I) IS THE INDEPENDENT
C     VARIABLE X, THE SECOND COLUMN IS THE STEADY-STATE,
C     AND THE REMAINING 8 COLUMNS ARE RESPONSES.
   37 X=AA
      DO 70 I=1,NV
      X=X+DELTX
      U(I)=X
      U(I+10)=F(I)
   70 CONTINUE
C
C     CALCULATE TRANSIENT SOLUTION MATRIX UT(X,T)
C
C     SET TIME-SPACE GRID
      IJK=20
```

```
      T=TL
      NTC=NT-1
      DO 71 I=1,NTC
      T=T+DELTT
      X=AA
      DO 72 J=1,NV
      X=X+DELTX
C
C     TIME-SPACE GRID NOW SET
C
C     SUM SERIES FOR EACH VALUE
      IJK=IJK+1
      UT(IJK)=0.0
      DO 73 K=1,NV
      IX=J+NV*(K-1)
      EXT=EXP(-TLAM(K)*T)
      UT(IJK)=UZ(K)*XI(IX)*EXT+UT(IJK)
   73 CONTINUE
      U(IJK)=US(J)+UT(IJK)
   72 CONTINUE
   71 CONTINUE
      RETURN
      END
```

```
$JOB            HAYES,KP=29,TIME=2,PAGES=50
C
C      MAIN PROGRAM TO USE PLPBV AS A TEST
       DIMENSION BC(10),U(100),US(10),UT(100),F(10)
       DIMENSION P(3),Q(3),A(2,4),PRMT(20)
       COMMON /S/P,Q,M
C
C          PLPBV INPUT SECTION
       M=3
       READ(5,100)(P(I),Q(I),I=1,M)
  100  FORMAT(2F10.5)
       READ(5,101)((A(I,J),J=1,4),I=1,2)
  101  FORMAT(4F10.5)
       READ(5,102)(PRMT(I),I=1,10)
  102  FORMAT(2E15.7)
       BC(7)=A(1,1)
       BC(9)=A(1,2)
       BC(1)=A(1,4)
       BC(4)=A(2,1)
       BC(6)=A(2,2)
       BC(2)=A(2,4)
C
C      SET UP LINEAR STEADY-STATE AS A TEST
       X=0.0
       DO 10 KSS=1,10
       F(KSS)=0.0
       X=X+0.1
       US(KSS)=X
   10  CONTINUE
C
C      TEST STEADY-STATE INPUT FOR PLPBV FROM UC1,APPENDIX A4
       PRMT(11)=0.06
       PRMT(12)=0.126
       PRMT(13)=0.200
       PRMT(14)=0.27
       PRMT(15)=0.37
       PRMT(16)=0.47
       PRMT(17)=0.59
       PRMT(18)=0.71
       PRMT(19)=0.84
       PRMT(20)=1.00
       CALL PLPBV(PRMT,P,Q,M,BC,F,US,UT,U)
       CALL EXIT
       END
```

SECTION 6

BIBLIOGRAPHY AND REFERENCING (B)

B1 BIBLIOGRAPHY

B2 BIBLIOGRAPHY REFERENCES LISTED BY AREA OF APPLICATION

B3 BIOGRAPHICAL NOTE

AN UNDERSTATEMENT:

" THE LITERATURE ON DISTILLATION IS VOLUMINOUS - "

R. J. HENGSTEBECK (H-18)

ONE OF THE MAJOR EFFORTS OF THIS THESIS TURNED OUT TO BE THE COMPILATION OF THE BIBLIOGRAPHY PRESENTED IN THIS SECTION. THE REFERENCES LISTED APPLY TO FOUR MAJOR AREAS PERTINENT TO THIS THESIS.

1. GENERAL THEORY OF DISTILLATION
2. DISTILLATION COLUMN DYNAMICS
3. DISTILLATION COLUMN CONTROL
4. MATHEMATICS AND COMPUTATION

THE AUTHOR HOPES THAT UTILIZATION OF CHAPTER B2, BIBLIOGRAPHY REFERENCES LISTED BY AREA OF APPLICATION, WILL RESULT IN CONSIDERABLE SAVINGS OF SEARCHING TIME AND EFFORT FOR ANYONE INTERESTED IN THESE AREAS.

CHAPTER B1

BIBLIOGRAPHY

This chapter presents a bibliography of 352 references pertinent to the general area of distillation and to the specific areas of this thesis. The references consist only of those in English, although extensive literature on distillation has been published in the foreign journals, especially in Russian and German. For the most part, the references were taken from the following journals for the years from about 1955 to 1969.

1. Industrial and Engineering Chemistry
2. American Institute of Chemical Engineers
3. Chemical Engineering Progress (and Symposium Series)
4. Transactions of the Institution of Chemical Engineers
5. Chemical Engineering Science
6. British Chemical Engineering
7. Canadian Journal of Chemical Engineering

The entries in this bibliography are in the order of the first letter of the author's last name, for the reader's mnemonic convenience, but no attempt has been made to subalphabetize within each group for this author's convenience.

It is this author's intention that Chapter B2 - Bibliography References Listed by Area of Application be used in conjunction with this chapter for any given subject or area of research. In each reference in this bibliography an attempt has been made, especially with journal articles, to present as complete a description as possible of

the reference, even at the cost of complete overspecification and possible redundancy of information.

The criterion of availability of each reference in the M.I.T. libraries (except for theses) placed a significant constraint on the number of references which have been listed here. The author chose this as his stopping point in the compilation of this bibliography.

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CHAPTER B2

BIBLIOGRAPHY REFERENCES LISTED BY AREA OF APPLICATION

The purpose of this chapter is to classify the references in Chapter B1, the Bibliography, according to their principal areas of application. The general format of this classification is presented in Table B2.1. Many of the references apply to more than one area and are so listed for the user's convenience. Rather than merely list the references under each area in alphabetical order, the author has chosen to present them column by column in the order of decreasing utility to the study of the subject or of decreasing clarity. In other words, the first listed in each area seem to the author to be the most important for anyone researching that area. Recognizing that such a listing is, indeed, very subjective, the author apologizes to anyone who may find them "out of order" with respect to his particular slant on the subject.

B2.1 General Theory of Distillation

Textbooks

Extensive Bibliographies and Literature Surveys

References of Historical Interest

General Distillation

Dynamic or Transient Analyses

Steady-State Analysis and McCabe-Thiele Diagrams

Structural Design

Economics and Operations Analysis

Thermodynamics

Hydrodynamics

Chemistry

Philosophy

Table B2.1 (Contd.)

B2.2 Distillation Column Dynamics

Textbooks

Theses

Reviews, Bibliographies, and Literature Surveys

Dynamic Models or Solutions

Discrete Plate Equations

Frequency Analysis or Laplace Transform Solution

Transient or Time Analysis

Numerical Solution

Digital Computer

Hybrid Computer

Analog Computer

Analytical Analysis

Continuous Spatial Equations

Frequency Analyses or Laplace Transform Solution

Transient or Time Analysis

Experimental Transient Behavior

Frequency Response

Time Response

Cyclic Distillation

B2.3 Distillation Column Control

Textbooks

Theses

Extensive Bibliographies and Literature Surveys

Conventional Control Systems

Digital Control

Hybrid Control

Table B2.1 (Contd.)

Analog Control

Instrumentation

Control Systems Using Dynamic Models

Digital Computer Control

Hybrid Computer Control

Analog Computer Control

Optimal Control

Distributed or Modal Control

B2.4 Mathematics and Computation

Ordinary Differential Equation Theory

Partial Differential Equation Theory

Integral Equation Theory

Mathematical Transformations

Matrix Mathematics

Numerical Solution Techniques

Boundary Value Problems

Eigen - Values, Vectors, and Functions

Special Functions

Computation and Computer Programming

Table B2.1 - FORMAT FOR CLASSIFICATION BY AREA OF APPLICATION

B2.1 GENERAL THEORY OF DISTILLATION

Textbooks

(B-1) (A-19) (H-18) (R-22) (T-1)

(G-3) (B-15) (L-26) (R-17) (B-12)

(H-10) (M-14) (C-5) (S-8) (H-5)

(R-23) (O-2) (C-1) (S-9) (C-7)

(R-21) (H-2) (P-3) (S-3) (M-2)

(V-2) (H-9) (P-10) (S-1) (V-3)

Extensive Bibliographies and Literature Surveys

(W-16) (G-9) (W-13) (W-18) (F-6)

(B-17) (R-12) (W-15) (W-26) (G-14)

(B-18) (P-11) (F-7) (Z-3) (W-23)

(B-19) (R-8) (R-25) (W-8)

(W-10) (H-7) (R-18) (W-17)

(W-11) (W-9) (H-8) (G-10)

(F-8) (W-12) (R-17) (W-19)

References of Historical Interest

General Distillation

(L-19) (L-25) (V-2) (E-3) (P-12) (G-14) (A-17)

(M-10) (M-9) (R-29) (C-15) (T-6) (I-1) (U-1)

Dynamic or Transient Analysis

(M-8) (B-29) (L-2) (B-7) (R-2) (R-12) (J-1) (F-5)

Steady State Analysis and McCabe - Thiele Diagrams

(B-1) (H-22) (C-1) (R-21) (S-23) (L-25) (S-7) (R-18)

(M-10) (B-10) (F-3) (H-30) (S-12) (R-30) (S-29) (A-19)

(E-4) (M-18) (F-4) (J-7) (C-14) (T-1) (W-30) (P-12)

(H-10) (P-8) (V-2) (L-12) (D-2) (E-2) (F-9) (T-7)

Steady State Analysis and McCabe - Thiele Diagrams (Contd.)

(H-18) (V-2) (F-15) (A-10) (O-2) (S-15) (E-1) (R-1)
(H-26) (S-15) (G-3) (A-17) (T-6) (S-5) (H-21) (R-29)
(C-9) (S-20) (H-5) (B-24) (P-13) (S-3) (I-1) (S-16)
(M-8) (Z-2) (H-2) (B-26) (R-5) (S-24) (L-24) (S-1)
(M-9) (R-26)

Structural Design

(L-13) (R-22) (F-10) (J-3) (M-11) (L-12) (D-11)

Economics and Operations Analysis

(L-15) (M-13) (B-15) (S-8) (F-9) (F-10) (C-7) (V-3)

Thermodynamics

(H-9) (R-23)

Hydrodynamics or Fluid Mechanics

(F-4) (V-2) (R-23) (S-5) (P-9) (B-4) (S-19)
(L-26) (B-12) (H-14) (G-11) (F-5) (M-24) (T-7)

Chemistry

(B-16) (B-1) (H-17) (T-6) (S-5) (R-23)
(H-8) (H-10) (F-9) (G-8) (H-20) (T-6)

Philosophy

(A-13) (B-28)

B2.2 DISTILLATION COLUMN DYNAMICS

Textbooks

(M-1) (H-7) (G-3) (F-16)

Theses

(F-14) (W-21) (D-14) (C-10) (B-32) (W-22) (S-27)
(M-15) (M-12) (M-17) (Q-1) (O-3) (G-5) (W-20)
(S-28) (A-5) (R-6) (R-27) (S-22) (M-19) (W-24)
(S-17) (C-4) (A-16) (L-17) (S-18) (M-24)

Reviews, Bibliographies, and Literature Surveys

(A-3) (H-7) (R-25) (W-15) (Z-3) (S-33) (L-3)
(R-12) (B-17) (R-8) (W-12) (G-9) (W-13) (T-2)
(W-16) (B-18) (W-10) (W-11) (B-19) (W-24) (W-23)

Dynamic Models or Solutions

Discrete Plate Equations

Frequency Analysis or Laplace Transform Solution

(A-3) (H-7) (R<25) (W-15) (Z-3) (S-33) (L-3)
(R-12) (B-17) (R-8) (W-12) (G-9) (W-13) (T-2)
(W-16) (B-18) (W-10) (W-11) (B-19) (W-24 (W-23)

Transient or Time Analysis

Numerical Solution

Digital Computer

(D-4) (R-16) (P-2) (T-9) (S-16)
(B-32) (R-9) (R-17) (W-25) (R-19)
(R-2) (A-4) (D-9) (Y-1) (L-27)
(D-8) (M-3) (L-18) (P-5) (S-20)
(H-3) (R-10) (D-6) (G-4) (W-4)
(L-5) (R-11) (A-9) (R-5) (R-18)
(R-20) (T-2) (S-6) (D-11)
(D-15) (W-1) (S-33) (R-1)

Hybrid Computer

(F-1) (F-13) (R-6) (F-12)

Analog Computer

(B-23) (P-1) (R-3) (G-12) (L-5)

Analytical Analysis

(D-3) (M-1) (S-31) (B-27) (H-20)

(G-2) (R-7) (W-2) (C-2) (H-21)

(A-3) (R-8) (F-16) (Z-3) (B-7)

(M-8) (R-32) (G-3) (F-5) (B-12)

Continuous Spatial Equations

Frequency Analysis or Laplace Transform Solution

(J-6) (M-27) (H-4) (S-7) (W-5) (D-1)

Transient or Time Analysis

(J-1) (R-8) (M-1) (L-26) (T-5) (J-5) (W-14)

(H-4) (D-3) (M-28) (P-7) (G-3) (L-20) (B-25)

(K-2) (S-13) (K-3) (R-14) (H-25) (B-20) (C-8)

(O-1) (D-14) (C-2) (B-29) (J-2) (B-24)

Experimental Transient Behavior

Frequency Response

(H-15) (H-23) (A-6) (H-24) (W-28)

Time Response

(H-3) (L-5) (B-5) (B-3) (R-15) (S-4) (D-12) (R-30)

Cyclic Distillation

(M-19) (A-14) (M-20) (B-17) (B-18) (S-4)

B2.3 DISTILLATION COLUMN CONTROL

Textbooks

(A-12) (G-3) (B-13) (K-5) (C-1) (C-15) (A-11) (L-1)

Theses

(B-2) (B-32) (M-5) (G-1) (S-18) (M-25)

Extensive Bibliographies and Literature Surveys

(A-3) (B-17) (R-25) (R-12) (W-10) (W-20) (W-12) (W-21)

(W-16) (B-18) (R-8) (S-33) (W-11) (B-19) (W-15) (W-23)

Conventional Control Systems

Digital Control

(S-32) (H-29) (B-6) (L-15) (L-24) (T-8)

Hybrid Control

(F-13) (F-1) (F-12)

Analog Control and Instrumentation

(H-16) (L-16) (B-10) (C-15) (G-12) (S-30) (M-29) (S-9)

(R-31) (B-13) (B-31) (P-6) (K-4) (C-12) (P-14) (W-23)

(G-3) (B-22) (C-1) (S-1) (L-4) (T-11) (R-13) (H-1)

Control Systems Using Dynamic Models

Digital Computer Control

(A-12) (D-4) (R-20) (L-18) (D-6) (S-33) (C-11) (W-18)

Hybrid Computer Control

(D-13) (A-8)

Analog Computer Control

(J-6) (L-14) (L-6) (W-27) (H-15) (K-2) (L-3) (R-3)

Optimal Control

(L-9) (B-32) (D-13) (A-8) (S-33) (J-5)

(B-11) (A-11) (K-5) (W-29)

Distributed or Modal Control

(D-9) (J-6) (M-5) (S-31) (C-4) (S-2) (F-16) (G-13)

B2.4 MATHEMATICS AND COMPUTATION

Ordinary Dirrerential Equation Theory

(H-11) (S-21) (B-14) (I-2) (H-12) (S-10) (H-6)

Partial Differential Equation Theory

(G-7) (B-21) (O-1) (F-16) (W-7)

(F-11) (A-15) (F-12) (G-6) (H-28)

Integral Equation Theory

(T-3) (L-8) (D-5) (S-11) (V-4) (T-10) (W-6)

(P-4) (H-13) (M-6) (S-14) (S-2) (G-7) (W-7)

Mathematical Transformations

(T-4) (Z-1) (S-31) (M-16) (R-14) (C-8)

Matrix Mathematics

(A-4) (A-12) (H-13) (J-7) (M-26)

Numerical Solution Techniques

(B-30) (F-11) (M-22) (P-5) (H-25) (D-9) (W-26)

(A-15) (K-1) (D-7) (A-10) (J-7) (D-10) (M-26)

(R-24) (L-10) (S-13) (R-4) (L-11) (M-2) (J-5)

(D-8) (L-1) (C-8) (P-8) (L-22) (N-1) (D-15)

(H-28) (L-21) (H-19) (R-29) (L-7) (R-17) (S-12)

(F-2) (B-32) (M-4) (P-12) (A-17) (T-10)

Boundary Value Problems

(L-11) (B-8) (S-10) (H-12) (L-7) (M-22)

(H-11) (B-14) (V-1) (H-25) (B-9) (P-5)

(K-1) (B-32) (F-2) (L-22) (C-6)

Eigen - Values, Vectors, and Functions

(B-30) (H-11) (B-14) (M-2) (S-31) (C-6) (J-7)

(A-12) (H-13) (C-13) (S-13) (V-1) (B-5)

(G-13) (I-2) (D-3) (S-10) (W-26) (H-12)

Special Functions

(A-18) (L-23) (M-16) (R-28) (H-27) (S-25) (S-26)

Computation and Computer Programming

(M-4) (I-3) (C-13) (M-18) (B-15)

(O-4) (P-8) (H-29) (S-32) (M-25)

CHAPTER B3

BIOGRAPHICAL NOTE

Lt. Michael N. Hayes was born in Abilene, Texas, on September 2, 1941. Four years later the family moved to Ohio, where he attended primary schools in Wakeman and in Massillon. He was graduated from Washington High School, Massillon, Ohio, in June 1959.

Mr. Hayes enlisted as a Seaman Recruit in the United States Navy in September, 1959. He was graduated from the U.S. Naval Guided Missiles School, Dam Neck, Virginia, in July, 1960, and was assigned to the U.S.S. Kitty Hawk (CVA-63) until June, 1961. He was graduated from the U.S. Naval Preparatory School, Bainbridge, Maryland, in August, 1961.

In September, 1961, Mr. Hayes began 4 years of undergraduate education at North Carolina State University, Raleigh, N.C., under the auspices of the Naval Enlisted Scientific Education Program (NESEP). He was graduated in June, 1965, with the degrees of Bachelor of Science in both Electrical Engineering and Applied Mathematics and with the degree of Master of Electrical Engineering.

After attending the U.S. Naval Officer Candidate School at Newport, R.I., Mr. Hayes was commissioned an Ensign in the U.S. Navy in October, 1965, and assigned for duty at the Boston Naval Shipyard, Boston, Massachusetts. While stationed at the Shipyard, he worked as a Ship Superintendent, supervising naval ship construction and repair, and attended evening classes at Boston University in business administration and at Northeastern University in pure mathematics.

In June, 1967, Mr. Hayes entered M.I.T. as a U.S. Naval Post-graduate student in Curriculum 13A with specialized studies in electrical engineering. He is a member of Tau Beta Pi, Eta Kappa Nu, Phi Eta Sigma, and is an Eagle Scout.

Lt. Hayes is married to the former Ann Marie Graney of Stoughton, Massachusetts. They have a one-year-old son, Stephen, and are expecting their second child in December, 1969.

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